

# O-nitro carbanilic acid, n-decyl ester

<b>Inchi:</b>	InChI=1S/C17H26N2O4/c1-2-3-4-5-6-7-8-11-14-23-17(20)18-15-12-9-10-13-16(15)19(21)
<b>InchiKey:</b>	CWFRDTPCZZHNOD-UHFFFAOYSA-N
<b>Formula:</b>	C17H26N2O4
<b>SMILES:</b>	CCCCCCCCCOC(=O)Nc1cccc1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	322.40
<b>CAS:</b>	93814-55-2

## Physical Properties

Property code	Value	Unit	Source
gf	86.06	kJ/mol	Joback Method
hf	-371.24	kJ/mol	Joback Method
hfus	52.68	kJ/mol	Joback Method
hvap	88.56	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.284		Crippen Method
mvol	261.470	ml/mol	McGowan Method
pc	1648.43	kPa	Joback Method
tb	898.32	K	Joback Method
tc	1116.00	K	Joback Method
tf	588.72	K	Joback Method
vc	1.020	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	829.31	J/mol×K	898.32	Joback Method
cpg	843.19	J/mol×K	934.60	Joback Method
cpg	855.96	J/mol×K	970.88	Joback Method
cpg	867.68	J/mol×K	1007.16	Joback Method
cpg	878.38	J/mol×K	1043.44	Joback Method
cpg	888.12	J/mol×K	1079.72	Joback Method
cpg	896.94	J/mol×K	1116.00	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=C93814552&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C93814552&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>

# 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>mcvol:</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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