

# O-nitro carbanilic acid, n-dodecyl ester

<b>Inchi:</b>	InChI=1S/C19H30N2O4/c1-2-3-4-5-6-7-8-9-10-13-16-25-19(22)20-17-14-11-12-15-18(17)
<b>InchiKey:</b>	HRTNGPYWIYRPMV-UHFFFAOYSA-N
<b>Formula:</b>	C19H30N2O4
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)Nc1ccccc1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	350.45
<b>CAS:</b>	94432-00-5

## Physical Properties

Property code	Value	Unit	Source
gf	102.90	kJ/mol	Joback Method
hf	-412.52	kJ/mol	Joback Method
hfus	57.87	kJ/mol	Joback Method
hvap	93.01	kJ/mol	Joback Method
log10ws	-6.99		Crippen Method
logp	6.064		Crippen Method
mcvol	289.650	ml/mol	McGowan Method
pc	1418.64	kPa	Joback Method
tb	944.08	K	Joback Method
tc	1163.02	K	Joback Method
tf	611.26	K	Joback Method
vc	1.133	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	947.24	J/molxK	944.08	Joback Method
cpg	961.51	J/molxK	980.57	Joback Method
cpg	974.62	J/molxK	1017.06	Joback Method
cpg	986.62	J/molxK	1053.55	Joback Method
cpg	997.56	J/molxK	1090.04	Joback Method
cpg	1007.50	J/molxK	1126.53	Joback Method
cpg	1016.50	J/molxK	1163.02	Joback Method

# Sources

<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.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=C94432005&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C94432005&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>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

Latest version available from:

<https://www.chemeo.com/cid/30-454-4/O-nitro-carbanilic-acid-n-dodecyl-ester.pdf>

Generated by Cheméo on 2024-04-23 11:14:26.99360523 +0000 UTC m=+16160115.914182580.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.