

# O-nitro carbanilic acid, thymol ester

<b>Inchi:</b>	InChI=1S/C17H18N2O4/c1-11(2)13-9-8-12(3)10-16(13)23-17(20)18-14-6-4-5-7-15(14)19
<b>InchiKey:</b>	XOBLYSKFOUACDO-UHFFFAOYSA-N
<b>Formula:</b>	C17H18N2O4
<b>SMILES:</b>	<chem>Cc1ccc(C(C)C)c(OC(=O)Nc2ccccc2[N+](=O)[O-])c1</chem>
<b>Mol. weight [g/mol]:</b>	314.34
<b>CAS:</b>	98309-55-8

## Physical Properties

Property code	Value	Unit	Source
gf	176.77	kJ/mol	Joback Method
hf	-162.93	kJ/mol	Joback Method
hfus	42.42	kJ/mol	Joback Method
hvap	91.77	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	4.638		Crippen Method
mcvol	237.710	ml/mol	McGowan Method
pc	2155.30	kPa	Joback Method
tb	934.52	K	Joback Method
tc	1184.51	K	Joback Method
tf	625.18	K	Joback Method
vc	0.906	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.59	J/molxK	934.52	Joback Method
cpg	735.28	J/molxK	976.19	Joback Method
cpg	745.68	J/molxK	1017.85	Joback Method
cpg	754.84	J/molxK	1059.52	Joback Method
cpg	762.83	J/molxK	1101.18	Joback Method
cpg	769.70	J/molxK	1142.85	Joback Method
cpg	775.51	J/molxK	1184.51	Joback Method

# Sources

<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=C98309558&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C98309558&amp;Units=SI</a>
<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>

# 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>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>mccol:</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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