

# p-Toluic acid, 4-nitrophenyl ester

<b>Other names:</b>	p-Toluylic acid, 4-nitrophenyl ester
<b>Inchi:</b>	InChI=1S/C14H11NO4/c1-10-2-4-11(5-3-10)14(16)19-13-8-6-12(7-9-13)15(17)18/h2-9H,
<b>InchiKey:</b>	IQTZVMBCINKMHK-UHFFFAOYSA-N
<b>Formula:</b>	C14H11NO4
<b>SMILES:</b>	<chem>Cc1ccc(C(=O)Oc2ccc([N+](=O)[O-])cc2)cc1</chem>
<b>Mol. weight [g/mol]:</b>	257.24

## Physical Properties

Property code	Value	Unit	Source
gf	74.19	kJ/mol	Joback Method
hf	-137.73	kJ/mol	Joback Method
hfus	33.47	kJ/mol	Joback Method
hvap	78.38	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	3.122		Crippen Method
mvol	185.460	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
rinpol	2206.00		NIST Webbook
rinpol	2206.00		NIST Webbook
tb	811.17	K	Joback Method
tc	1073.33	K	Joback Method
tf	541.19	K	Joback Method
vc	0.710	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.87	J/molxK	811.17	Joback Method
cpg	520.90	J/molxK	854.86	Joback Method
cpg	531.68	J/molxK	898.56	Joback Method
cpg	541.27	J/molxK	942.25	Joback Method
cpg	549.73	J/molxK	985.95	Joback Method
cpg	557.11	J/molxK	1029.64	Joback Method
cpg	563.48	J/molxK	1073.33	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U307770&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U307770&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>
<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>

# 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>hvp:</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>rinp:</b>	Non-polar retention indices
<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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