

# Carbanilic acid, 2-tert-butyl-, ethyl ester

<b>Inchi:</b>	InChI=1S/C13H19NO2/c1-5-16-12(15)14-11-9-7-6-8-10(11)13(2,3)4/h6-9H,5H2,1-4H3,(H
<b>InchiKey:</b>	JMCPSSGDDONVOA-UHFFFAOYSA-N
<b>Formula:</b>	C13H19NO2
<b>SMILES:</b>	CCOC(=O)Nc1ccccc1C(C)(C)C
<b>Mol. weight [g/mol]:</b>	221.30
<b>CAS:</b>	100096-59-1

## Physical Properties

Property code	Value	Unit	Source
gf	19.67	kJ/mol	Joback Method
hf	-286.67	kJ/mol	Joback Method
hfus	23.55	kJ/mol	Joback Method
hvap	61.77	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.552		Crippen Method
mcvol	187.690	ml/mol	McGowan Method
pc	2329.27	kPa	Joback Method
tb	651.73	K	Joback Method
tc	866.80	K	Joback Method
tf	402.45	K	Joback Method
vc	0.704	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.52	J/molxK	651.73	Joback Method
cpg	515.34	J/molxK	687.57	Joback Method
cpg	530.13	J/molxK	723.42	Joback Method
cpg	543.93	J/molxK	759.26	Joback Method
cpg	556.78	J/molxK	795.11	Joback Method
cpg	568.73	J/molxK	830.95	Joback Method
cpg	579.83	J/molxK	866.80	Joback Method

# Sources

<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>
<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=C100096591&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C100096591&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

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