

# Acetanilide, n-tert-butyl-

<b>Inchi:</b>	InChI=1S/C12H17NO/c1-10(14)13(12(2,3)4)11-8-6-5-7-9-11/h5-9H,1-4H3
<b>InchiKey:</b>	UGBHGSVEQNCPOY-UHFFFAOYSA-N
<b>Formula:</b>	C12H17NO
<b>SMILES:</b>	CC(=O)N(c1cccc1)C(C)(C)C
<b>Mol. weight [g/mol]:</b>	191.27
<b>CAS:</b>	91562-67-3

## Physical Properties

Property code	Value	Unit	Source
gf	147.27	kJ/mol	Joback Method
hf	-108.28	kJ/mol	Joback Method
hfus	18.08	kJ/mol	Joback Method
hvap	52.08	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.838		Crippen Method
mcvol	167.730	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
tb	563.72	K	Joback Method
tc	781.64	K	Joback Method
tf	336.24	K	Joback Method
vc	0.613	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.47	J/molxK	563.72	Joback Method
cpg	424.56	J/molxK	600.04	Joback Method
cpg	440.44	J/molxK	636.36	Joback Method
cpg	455.16	J/molxK	672.68	Joback Method
cpg	468.82	J/molxK	709.00	Joback Method
cpg	481.47	J/molxK	745.32	Joback Method
cpg	493.20	J/molxK	781.64	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=C91562673&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C91562673&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>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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