

# Acetanilide, 2-chloro-4-tert-butyl-

**Inchi:** InChI=1S/C12H16ClNO/c1-8(15)14-11-6-5-9(7-10(11)13)12(2,3)4/h5-7H,1-4H3,(H,14,15)  
**InchiKey:** NQEYFCHLAJWJIX-UHFFFAOYSA-N  
**Formula:** C12H16ClNO  
**SMILES:** CC(O)=Nc1ccc(C(C)(C)C)cc1Cl  
**Mol. weight [g/mol]:** 225.72  
**CAS:** 100141-30-8

## Physical Properties

Property code	Value	Unit	Source
hf	-181.71	kJ/mol	Joback Method
hvap	69.07	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	4.245		Crippen Method
mvol	179.970	ml/mol	McGowan Method
pc	2278.41	kPa	Joback Method
tb	713.54	K	Joback Method
tc	934.12	K	Joback Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C100141308&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## Legend

**hf:** Enthalpy of formation at standard conditions  
**hvap:** Enthalpy of vaporization at standard conditions  
**log10ws:** 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

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