# Acetanilide, 6-tert-butyl-2,4-dimethyl-

**Inchi:** InChI=1S/C14H21NO/c1-9-7-10(2)13(15-11(3)16)12(8-9)14(4,5)6/h7-8H,1-6H3,(H,15,16)
**InchiKey:** FVHRNYIVAVWDKU-UHFFFAOYSA-N
**Formula:** C14H21NO
**SMILES:** CC(O)=Nc1c(C)cc(C)cc1C(C)(C)C
**Mol. weight [g/mol]:** 219.32
**CAS:** 110491-71-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -218.72 | kJ/mol | Joback Method |
| hvap | 69.80 | kJ/mol | Joback Method |
| log10ws | -4.12 | | Crippen Method |
| logp | 4.209 | | Crippen Method |
| mcvol | 195.910 | ml/mol | McGowan Method |
| pc | 1949.23 | kPa | Joback Method |
| tb | 726.85 | K | Joback Method |
| tc | 938.78 | K | Joback Method |

## Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C110491719&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**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

| | |
|---|---|
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |