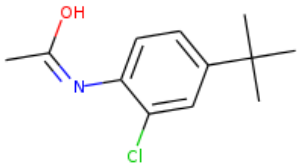
Acetanilide, 2-chloro-4-tert-butyl-

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)
InChI Key: NQEYFCHLAJWJIX-UHFFFAOYSA-N
Formula: C12H16ClNO
SMILES: CC(O)=Nc1ccc(C(C)(C)C)cc1Cl
Molecular Weight: 225.71
CAS: 100141-30-8



Physical Properties

Property	Value	Unit	Source
$\Delta_f H°_{gas}$	-181.71	kJ/mol	Joback Method
$\Delta_{vap} H°$	69.07	kJ/mol	Joback Method
$logP_{oct/wat}$	4.25		Crippen Method
P_c	2278.41	kPa	Joback Method
T_{boil}	713.54	K	Joback Method
T_c	934.12	K	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/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)
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{vap} H°$: Enthalpy of vaporization at standard conditions (kJ/mol).
$logP_{oct/wat}$: Octanol/Water partition coefficient .
P_c: Critical Pressure (kPa).
T_{boil}: Normal Boiling Point Temperature (K).

T_c: Critical Temperature (K).