

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)

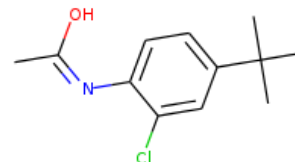
InChI Key: NQEYFCHLAJWJIX-UHFFFAOYSA-N

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
$\Delta_f H^\circ_{\text{gas}}$	-181.71	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	69.07	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	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,\(H,14,15\)](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/ci9903071>

Legend

$\Delta_f H^\circ_{\text{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{\text{vap}} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

P_c : Critical Pressure (kPa).

T_{boil} : Normal Boiling Point Temperature (K).

T_c : Critical Temperature (K).

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