Acetanilide, 2-tert-butyl-

Inchi: InChI=1S/C12H17NO/c1-9(14)13-11-8-6-5-7-10(11)12(2,3)4/h5-8H,1-4H3,(H,13,14)
InchiKey: HNFBHUKCHBRSSD-UHFFFAOYSA-N
Formula: C12H17NO
SMILES: CC(O)=Nc1ccccc1C(C)(C)C
Mol. weight [g/mol]: 191.27
CAS: 7402-70-2

Physical Properties

Property code	Value	Unit	Source
hf	-154.50	kJ/mol	Joback Method
hvap	64.02	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	3.592		Crippen Method
mcvol	167.730	ml/mol	McGowan Method
pc	2395.87	kPa	Joback Method
tb	671.13	K	Joback Method
tc	887.80	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7402702&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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