Acetanilide, n-tert-butyl-3-chloro-

Inchi: InChI=1S/C12H16ClNO/c1-9(15)14(12(2,3)4)11-7-5-6-10(13)8-11/h5-8H,1-4H3
InchiKey: AIXVBEWBQIYLGN-UHFFFAOYSA-N
Formula: C12H16ClNO
SMILES: CC(=O)N(c1cccc(Cl)c1)C(C)(C)C
Mol. weight [g/mol]: 225.72

Physical Properties

Property code	Value	Unit	Source
gf	125.71	kJ/mol	Joback Method
hf	-135.49	kJ/mol	Joback Method
hfus	21.89	kJ/mol	Joback Method
hvap	57.12	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	3.491		Crippen Method
mcvol	179.970	ml/mol	McGowan Method
pc	2472.73	kPa	Joback Method
tb	606.13	K	Joback Method
tc	828.96	K	Joback Method
tf	378.68	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.15	J/mol×K	606.13	Joback Method
cpg	451.68	J/mol×K	643.27	Joback Method
cpg	466.07	J/mol×K	680.41	Joback Method
cpg	479.40	J/mol×K	717.55	Joback Method
cpg	491.73	J/mol×K	754.68	Joback Method
cpg	503.15	J/mol×K	791.82	Joback Method
cpg	513.72	J/mol×K	828.96	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009290&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume