Aniline, n-tert-butyl-2-chloro-

Inchi: InChI=1S/C10H14ClN/c1-10(2,3)12-9-7-5-4-6-8(9)11/h4-7,12H,1-3H3
InchiKey: MPDOKHFNDKPACR-UHFFFAOYSA-N
Formula: C10H14ClN
SMILES: CC(C)(C)Nc1ccccc1Cl
Mol. weight [g/mol]: 183.68
CAS: 939-36-6

Physical Properties

Property code	Value	Unit	Source
gf	216.40	kJ/mol	Joback Method
hf	4.31	kJ/mol	Joback Method
hfus	17.19	kJ/mol	Joback Method
hvap	50.32	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.550		Crippen Method
mcvol	150.220	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
tb	544.23	K	Joback Method
tc	770.30	K	Joback Method
tf	326.40	K	Joback Method
vc	0.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.26	J/mol×K	544.23	Joback Method
cpg	351.24	J/mol×K	581.91	Joback Method
cpg	365.16	J/mol×K	619.59	Joback Method
cpg	378.07	J/mol×K	657.27	Joback Method
cpg	390.05	J/mol×K	694.94	Joback Method
cpg	401.14	J/mol×K	732.62	Joback Method
cpg	411.43	J/mol×K	770.30	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=C939366&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