4-t-Butylbenzeneamine

Other names:	4-(1,1-Dimethylethyl)benzenamine
	4-(t-Butyl)aniline
	4-Amino-tert-butylbenzene
	4-tert-Butylaniline
	4-tert-Butylbenzenamine
	4-tert-Butylbenzeneamine
	Aniline, 4-tert-butyl-
	Aniline, p-tert-butyl-
	Benzenamine, 4-(1,1-dimethylethyl)-
	p-t-Butylaniline
	p-tert-Butylaniline
Inchi:	InChI=1S/C10H15N/c1-10(2,3)8-4-6-9(11)7-5-8/h4-7H,11H2,1-3H3
InchiKey:	WRDWWAVNELMWAM-UHFFFAOYSA-N
Formula:	C10H15N
SMILES:	CC(C)(C)c1ccc(N)cc1
Mol. weight [g/mol]:	149.23
CAS:	769-92-6

Physical Properties

Property code	Value	Unit	Source
gf	205.39	kJ/mol	Joback Method
hf	0.37	kJ/mol	Joback Method
hfus	13.09	kJ/mol	Joback Method
hvap	50.14	kJ/mol	Joback Method
ie	7.70 ± 0.10	eV	NIST Webbook
ie	7.35 ± 0.02	eV	NIST Webbook
log10ws	-2.42		Crippen Method
logp	2.566		Crippen Method
mcvol	137.980	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
rinpol	1270.40		NIST Webbook
rinpol	1270.40		NIST Webbook
ripol	2011.00		NIST Webbook
tb	504.00 ± 1.00	K	NIST Webbook
tc	760.46	K	Joback Method
tf	327.08	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.50	J/mol×K	529.16	Joback Method
cpg	335.25	J/mol×K	567.71	Joback Method
cpg	349.89	J/mol×K	606.26	Joback Method
cpg	363.48	J/mol×K	644.81	Joback Method
cpg	376.10	J/mol×K	683.36	Joback Method
cpg	387.79	J/mol×K	721.91	Joback Method
cpg	398.65	J/mol×K	760.46	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	364.70	K	0.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57409e+01
Coeff. B	-4.67055e+03
Coeff. C	-8.40840e+01
Temperature range (K), min.	386.32
Temperature range (K), max.	531.91

Sources

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=C769926&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume