N,N-Dimethyl-4-t-butylbenzeneamine

Other names:	4-tert-Butyl-N,N-dimethylaniline Benzenamine, 4-(1,1-dimethylethyl)-N,N-dimethyl- p-t-Butyl-N,N-dimethylaniline p-tert-Butyl-N,N-dimethylaniline
Inchi:	InChI=1S/C12H19N/c1-12(2,3)10-6-8-11(9-7-10)13(4)5/h6-9H,1-5H3
InchiKey:	SJDILFZCXQHCRB-UHFFFAOYSA-N
Formula:	C12H19N
SMILES:	CN(C)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]:	177.29
CAS:	2909-79-7

Physical Properties

Property code	Value	Unit	Source
gf	266.56	kJ/mol	Joback Method
hf	-7.17	kJ/mol	Joback Method
hfus	16.10	kJ/mol	Joback Method
hvap	45.99	kJ/mol	Joback Method
ie	6.90 ± 0.02	eV	NIST Webbook
ie	7.43	eV	NIST Webbook
log10ws	-2.69		Crippen Method
logp	3.050		Crippen Method
mcvol	166.160	ml/mol	McGowan Method
pc	2410.00	kPa	Joback Method
tb	524.70	K	NIST Webbook
tb	493.15 ± 4.00	K	NIST Webbook
tc	725.24	K	Joback Method
tf	298.83	K	Joback Method
vc	0.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.78	J/mol×K	514.83	Joback Method
cpg	402.24	J/mol×K	549.90	Joback Method

cpg	419.51	J/mol×K	584.97	Joback Method
cpg	435.67	J/mol×K	620.03	Joback Method
cpg	450.78	J/mol×K	655.10	Joback Method
cpg	464.89	J/mol×K	690.17	Joback Method
cpg	478.08	J/mol×K	725.24	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48710e+01
Coeff. B	-4.48756e+03
Coeff. C	-8.70030e+01
Temperature range (K), min.	394.72
Temperature range (K), max.	556.44

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2909797&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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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