Benzenamine, N,N,4-trimethyl-

Other names:	1-(Dimethylamino)-4-methylbenzene
	4-DIMETHYLAMINOTOLUENE
	4-METHYL-N,N-DIMETHYLANILINE
	Benzeneamine,N,N,4-trimethyl-
	Dimethyl-p-toluidine
	Dimetil-p-toluidina
	N,N,4-Trimethylaniline
	N,N,4-Trimethylbenzenamine
	N,N-Dimethyl-4-methylaniline
	N,N-Dimethyl-4-toluidine
	N,N-Dimethyl-p-toluidine
	N,N-Dimethyl-p-tolylamine
	NSC 1785
	P-METHYLDIMETHYLANILINE
	p,N,N-trimethylaniline
	p-(Dimethylamino)toluene
	p-Methyl-N,N-dimethylaniline
	p-Toluidine, N,N-dimethyl-
Inchi:	InChI=1S/C9H13N/c1-8-4-6-9(7-5-8)10(2)3/h4-7H,1-3H3
InchiKey:	GYVGXEWAOAAJEU-UHFFFAOYSA-N
Formula:	C9H13N
SMILES:	Cc1ccc(N(C)C)cc1
Mol. weight [g/mol]:	135.21
CAS:	99-97-8

Physical Properties

Property code	Value	Unit	Source
affp	950.00	kJ/mol	NIST Webbook
basg	918.10	kJ/mol	NIST Webbook
chl	-5411.20 ± 2.40	kJ/mol	NIST Webbook
gf	238.46	kJ/mol	Joback Method
hf	68.90 ± 7.40	kJ/mol	NIST Webbook
hfl	11.70 ± 2.70	kJ/mol	NIST Webbook
hfus	15.74	kJ/mol	Joback Method
hvap	57.20 ± 6.90	kJ/mol	NIST Webbook
hvap	57.20	kJ/mol	NIST Webbook
ie	7.33	eV	NIST Webbook

ie	7.48	eV	NIST Webbook
ie	6.93 ± 0.02	eV	NIST Webbook
ie	6.93	eV	NIST Webbook
ie	6.95 ± 0.05	eV	NIST Webbook
ie	6.90 ± 0.10	eV	NIST Webbook
ie	6.95	eV	NIST Webbook
ie	7.27	eV	NIST Webbook
log10ws	-1.86		Crippen Method
logp	2.061		Crippen Method
mcvol	123.890	ml/mol	McGowan Method
pc	3199.16	kPa	Joback Method
rinpol	1162.00		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1160.40		NIST Webbook
rinpol	1160.40		NIST Webbook
ripol	1642.60		NIST Webbook
ripol	1673.90		NIST Webbook
ripol	1673.90		NIST Webbook
tb	484.20	K	NIST Webbook
tb	483.15 ± 2.00	K	NIST Webbook
tb	484.30 ± 1.00	K	NIST Webbook
tc	655.29	K	Joback Method
tf	262.60	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.58	J/mol×K	620.98	Joback Method
cpg	246.45	J/mol×K	449.42	Joback Method
cpg	261.05	J/mol×K	483.73	Joback Method
cpg	274.83	J/mol×K	518.04	Joback Method
cpg	287.83	J/mol×K	552.35	Joback Method
cpg	300.07	J/mol×K	586.67	Joback Method
cpg	322.41	J/mol×K	655.29	Joback Method
hvapt	60.70	kJ/mol	403.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.18799e+02
Coeff. B	-1.10023e+04
Coeff. C	-1.51292e+01
Coeff. D	9.00408e-06
Temperature range (K), min.	323.15
Temperature range (K), max.	483.15

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
KDB: https://www.cheric.org/files/research/kdb/mol/mol1486.mol
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C99978&Units=SI
KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1486
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp: Proton affinity
basg: Gas basicity
chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume