

Benzenamine, N,N,3-trimethyl-

Other names:	m-Toluidine, N,N-dimethyl- m-Methyl-N,N-dimethylaniline m,N,N-trimethylaniline Benzene, 1-(dimethylamino)-3-methyl- Dimethyl-m-toluidine N,N-Dimethyl-m-methylaniline N,N-Dimethyl-m-toluidine N,N-Dimethyl-3-methylaniline N,N,3-Trimethylaniline N,N,3-Trimethylbenzenamine N,N-Dimethyl-3-toluidine Dimetil-m-toluidina Benzeneamine,N,N,3-trimethyl- 3-(Dimethylamino)toluene NSC 1788 N,N-Dimethyl-m-ethylaniline
Inchi:	InChI=1S/C9H13N/c1-8-5-4-6-9(7-8)10(2)3/h4-7H,1-3H3
InchiKey:	CWOMTHDOJCARBY-UHFFFAOYSA-N
Formula:	C9H13N
SMILES:	Cc1cccc(N(C)C)c1
Mol. weight [g/mol]:	135.21
CAS:	121-72-2

Physical Properties

Property code	Value	Unit	Source
affp	942.10	kJ/mol	NIST Webbook
basg	915.70	kJ/mol	NIST Webbook
chl	-5413.90 ± 2.20	kJ/mol	NIST Webbook
gf	238.46	kJ/mol	Joback Method
hf	72.60 ± 7.30	kJ/mol	NIST Webbook
hfl	14.40 ± 2.50	kJ/mol	NIST Webbook
hfus	15.74	kJ/mol	Joback Method
hvap	58.20	kJ/mol	NIST Webbook
hvap	58.20 ± 6.90	kJ/mol	NIST Webbook
hvap	58.20 ± 6.90	kJ/mol	NIST Webbook
ie	7.06	eV	NIST Webbook
ie	7.27	eV	NIST Webbook

ie	7.24	eV	NIST Webbook
ie	7.35	eV	NIST Webbook
ie	7.24	eV	NIST Webbook
ie	7.02	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	1164.60		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1174.00		NIST Webbook
ripol	1653.20		NIST Webbook
ripol	1653.60		NIST Webbook
ripol	1664.00		NIST Webbook
tb	488.20	K	NIST Webbook
tb	485.20	K	NIST Webbook
tb	486.50 ± 1.50	K	NIST Webbook
tc	655.29	K	Joback Method
tf	262.60	K	Joback Method
vc	0.450	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	311.58	J/mol×K	620.98	Joback Method
cpg	322.41	J/mol×K	655.29	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C121722&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical 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

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