Benzenamine, 3-methyl-

Other names:	1-Amino-3-methylbenzene
	3-Amino-1-methylbenzene
	3-Aminophenylmethane
	3-Aminotoluen
	3-Aminotoluene
	3-METHYLBENZENEAMINE
	3-Methylaniline
	3-Methylbenzenamine
	3-Toluidine
	3-methyl-benzamine
	Aniline, 3-methyl-
	M-AMINOTOLUENE
	M-METHYLANILINE
	NSC 15349
	benzeneamine, 3-methyl-
	m-Methylbenzenamine
	m-Toluidin
	m-Toluidine
	m-Tolylamine
Inchi:	InChI=1S/C7H9N/c1-6-3-2-4-7(8)5-6/h2-5H,8H2,1H3
InchiKey:	JJYPMNFTHPTTDI-UHFFFAOYSA-N
Formula:	C7H9N
SMILES:	Cc1cccc(N)c1
Mol. weight [g/mol]:	107.15
CAS:	108-44-1

Physical Properties

Property code	Value	Unit	Source
affp	895.80	kJ/mol	NIST Webbook
basg	864.00	kJ/mol	NIST Webbook
chl	-4047.00	kJ/mol	NIST Webbook
chl	-4083.00	kJ/mol	NIST Webbook
gf	177.29	kJ/mol	Joback Method
hf	61.10	kJ/mol	NIST Webbook
hf	87.90	kJ/mol	NIST Webbook
hfl	42.30	kJ/mol	NIST Webbook
hfus	12.73	kJ/mol	Joback Method

hvap	45.61	kJ/mol	NIST Webbook
hvap	56.40	kJ/mol	NIST Webbook
hvap	59.60 ± 0.30	kJ/mol	NIST Webbook
hvap	62.70 ± 0.50	kJ/mol	NIST Webbook
hvap	64.10	kJ/mol	NIST Webbook
hvap	58.30 ± 0.40	kJ/mol	NIST Webbook
ie	7.66	eV	NIST Webbook
ie	7.54 ± 0.03	eV	NIST Webbook
ie	7.75	eV	NIST Webbook
ie	7.66	eV	NIST Webbook
ie	7.60 ± 0.10	eV	NIST Webbook
ie	7.55	eV	NIST Webbook
ie	7.50 ± 0.02	eV	NIST Webbook
ie	7.70 ± 0.10	eV	NIST Webbook
ie	7.82	eV	NIST Webbook
log10ws	-0.85		Aqueous Solubility Prediction Method
log10ws	-0.85		Estimated Solubility Method
logp	1.577		Crippen Method
mcvol	95.710	ml/mol	McGowan Method
pc	4280.00	kPa	KDB
pc	4154.33 ± 303.98	kPa	NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	177.34		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1047.50		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	177.34		NIST Webbook
ripol	1840.00		NIST Webbook
ripol	1831.00		NIST Webbook
ripol	1831.00		NIST Webbook
ripol	1853.00		NIST Webbook
ripol	1838.00		NIST Webbook

ripol	1849.00		NIST Webbook
ripol	1840.00		NIST Webbook
ripol	1835.00		NIST Webbook
ripol	1840.00		NIST Webbook
tb	476.15 ± 1.00	K	NIST Webbook
tb	472.20 ± 1.00	K	NIST Webbook
tb	476.30 ± 0.40	K	NIST Webbook
tb	476.40 ± 0.50	K	NIST Webbook
tb	476.01 ± 0.20	K	NIST Webbook
tb	476.35 ± 0.30	K	NIST Webbook
tb	476.15 ± 0.50	K	NIST Webbook
tb	476.55 ± 0.30	K	NIST Webbook
tb	476.25 ± 0.30	K	NIST Webbook
tb	476.49 ± 0.07	K	NIST Webbook
tb	476.50	K	NIST Webbook
tb	476.52	K	KDB
tb	471.90 ± 0.50	K	NIST Webbook
tb	476.25 ± 0.40	K	NIST Webbook
tc	707.00	K	KDB
tc	709.15 ± 2.00	K	NIST Webbook
tf	242.15 ± 0.40	K	NIST Webbook
tf	241.70 ± 0.50	K	NIST Webbook
tf	242.72	K	Aqueous Solubility Prediction Method
tf	242.00 ± 0.30	K	NIST Webbook
tf	242.80 ± 0.02	K	NIST Webbook
tf	229.60 ± 0.60	K	NIST Webbook
tf	241.90 ± 0.30	K	NIST Webbook
tf	242.75 ± 0.05	K	NIST Webbook
tf	241.90 ± 0.10	K	NIST Webbook
tf	241.70 ± 1.50	K	NIST Webbook
tf	241.90	K	KDB
vc	0.348	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.04	J/mol×K	463.75	Joback Method
cpg	199.40	J/mol×K	501.76	Joback Method
cpg	210.07	J/mol×K	539.77	Joback Method
cpg	220.08	J/mol×K	577.78	Joback Method

cpg	229.46	J/mol×K	615.79	Joback Method
cpg	238.23	J/mol×K	653.80	Joback Method
cpg	246.42	J/mol×K	691.81	Joback Method
cpl	167.20	J/mol×K	303.15	NIST Webbook
cpl	216.70	J/mol×K	302.70	NIST Webbook
cpl	216.70	J/mol×K	302.70	NIST Webbook
hfust	8.80	kJ/mol	241.65	NIST Webbook
hfust	8.80	kJ/mol	241.70	NIST Webbook
hfust	8.80	kJ/mol	241.70	NIST Webbook
hvapt	51.10	kJ/mol	435.50	NIST Webbook
sfust	36.00	J/mol×K	241.65	NIST Webbook
speedsl	1567.00	m/s	303.15	Thermodynamic and acoustic properties of binary mixtures of ethers. III. Diisopropyl ether or oxolane with o- or m-toluidines at 303.15, 313.15 and 323.15 K
speedsl	1533.00	m/s	313.15	Thermodynamic and acoustic properties of binary mixtures of ethers. III. Diisopropyl ether or oxolane with o- or m-toluidines at 303.15, 313.15 and 323.15 K
speedsl	1492.00	m/s	323.15	Thermodynamic and acoustic properties of binary mixtures of ethers. III. Diisopropyl ether or oxolane with o- or m-toluidines at 303.15, 313.15 and 323.15 K

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43802e+01

Coeff. B	-3.58551e+03
Coeff. C	-1.08703e+02
Temperature range (K), min.	363.13
Temperature range (K), max.	504.07

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.48797e+01
Coeff. B	-8.59789e+03
Coeff. C	-6.91816e+00
Coeff. D	1.91528e-06
Temperature range (K), min.	242.75
Temperature range (K), max.	709.15

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108441&Units=SI
Thermodynamic and acoustic properties of binary mixtures of ethers. II. Diisopropyl ether or oxolane with o-toluidines at 303.15, 313.15 and 323.15 K:	https://www.doi.org/10.1016/j.tca.2011.01.019
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1298.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1298
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume