Methylamine, N,N-dimethyl-

Other names:	Methanamine, N,N-dimethyl- N,N-DIMETHYL-METHYLAMINE N,N-dimethylmethanamine TMA Trimethylamine UN 1083 UN 1297
Inchi:	InChI=1S/C3H9N/c1-4(2)3/h1-3H3
InchiKey:	GETQZCLCWQTVFV-UHFFFAOYSA-N
Formula:	C3H9N
SMILES:	CN(C)C
Mol. weight [g/mol]:	59.11
CAS:	75-50-3

Physical Properties

Property code	Value	Unit	Source
af	0.2050		KDB
affp	948.90	kJ/mol	NIST Webbook
basg	918.10	kJ/mol	NIST Webbook
chl	-2484.00	kJ/mol	NIST Webbook
chl	-2430.00	kJ/mol	NIST Webbook
dm	0.60	debye	KDB
gf	98.98	kJ/mol	KDB
gyrad	2.7360		KDB
hf	-23.70 ± 0.75	kJ/mol	NIST Webbook
hf	-23.86	kJ/mol	KDB
hf	-30.70	kJ/mol	NIST Webbook
hfl	-45.73 ± 0.71	kJ/mol	NIST Webbook
hfl	-52.70	kJ/mol	NIST Webbook
hfus	6.55	kJ/mol	Joback Method
hvap	22.18	kJ/mol	NIST Webbook
hvap	22.00 ± 0.08	kJ/mol	NIST Webbook
hvap	22.00	kJ/mol	NIST Webbook
ie	8.54	eV	NIST Webbook
ie	8.50	eV	NIST Webbook
ie	8.45 ± 0.01	eV	NIST Webbook
ie	7.85 ± 0.05	eV	NIST Webbook

ie	7.80	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	7.80 ± 0.10	eV	NIST Webbook
ie	7.88	eV	NIST Webbook
ie	7.83 ± 0.05	eV	NIST Webbook
ie	7.83 ± 0.02	eV	NIST Webbook
ie	7.95 ± 0.10	eV	NIST Webbook
ie	7.80	eV	NIST Webbook
ie	8.50 ± 0.10	eV	NIST Webbook
ie	8.54	eV	NIST Webbook
ie	8.47	eV	NIST Webbook
ie	8.45	eV	NIST Webbook
ie	8.44	eV	NIST Webbook
ie	8.56	eV	NIST Webbook
ie	7.82 ± 0.02	eV	NIST Webbook
log10ws	0.84		Aqueous Solubility Prediction Method
logp	0.178		Crippen Method
mcvol	63.110	ml/mol	McGowan Method
nfpaf	%!d(float64=4)		KDB
nfpah	%!d(float64=2)		KDB
pc	4087.00	kPa	KDB
pc	4087.00 ± 3.00	kPa	NIST Webbook
pc	4077.12 ± 10.66	kPa	NIST Webbook
rinpol	479.00		NIST Webbook
rinpol	479.00		NIST Webbook
rinpol	503.00		NIST Webbook
rinpol	518.00		NIST Webbook
ripol	609.00		NIST Webbook
ripol	561.00		NIST Webbook
ripol	570.00		NIST Webbook
ripol	576.00		NIST Webbook
ripol	554.00		NIST Webbook
ripol	546.00		NIST Webbook
ripol	570.00		NIST Webbook
ripol	609.00		NIST Webbook
ripol	553.00		NIST Webbook
ripol	570.00		NIST Webbook
ripol	610.00		NIST Webbook
sl	197.82	J/mol×K	NIST Webbook
tb	276.02	K	KDB
tc	433.20	K	NIST Webbook
tc	432.79 ± 0.15	K	NIST Webbook
tc	432.79	K	KDB
tc	433.30 ± 0.30	K	NIST Webbook

tf	155.95 ± 2.00	K	NIST Webbook
tf	156.00	K	KDB
tf	149.40 ± 0.50	K	NIST Webbook
tf	156.11	K	Aqueous Solubility Prediction Method
tf	155.95 ± 0.20	K	NIST Webbook
tf	155.85 ± 0.50	K	NIST Webbook
tf	149.15 ± 1.00	K	NIST Webbook
tt	156.08 ± 0.05	K	NIST Webbook
vc	30.000 ± 0.070	m3/kmol	NIST Webbook
vc	0.254	m3/kmol	KDB
zc	0.2884860		KDB
zra	0.27		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	86.78	J/mol×K	280.48	Joback Method
cpg	121.39	J/mol×K	413.32	Joback Method
cpg	114.99	J/mol×K	386.75	Joback Method
cpg	108.34	J/mol×K	360.18	Joback Method
cpg	101.42	J/mol×K	333.61	Joback Method
cpg	94.24	J/mol×K	307.05	Joback Method
cpg	127.54	J/mol×K	439.88	Joback Method
cpl	132.55	J/mol×K	280.00	NIST Webbook
hfust	6.54	kJ/mol	156.10	NIST Webbook
hfust	6.54	kJ/mol	156.08	NIST Webbook
hvapt	24.10	kJ/mol	276.00	KDB
hvapt	24.35	kJ/mol	276.20	NIST Webbook
hvapt	24.50	kJ/mol	250.00	NIST Webbook
hvapt	22.94 ± 0.03	kJ/mol	276.03	NIST Webbook
hvapt	24.10	kJ/mol	293.00	NIST Webbook
hvapt	23.00	kJ/mol	368.00	NIST Webbook
hvapt	24.60	kJ/mol	234.50	NIST Webbook
hvapt	22.94	kJ/mol	276.00	NIST Webbook
hvapt	22.94	kJ/mol	276.03	NIST Webbook
rhol	633.00	kg/m3	293.00	KDB
sfust	41.93	J/mol×K	156.08	NIST Webbook
srf	0.01	N/m	293.20	KDB
svapt	83.10	J/mol×K	276.03	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41103e+01
Coeff. B	-2.28172e+03
Coeff. C	-3.46150e+01
Temperature range (K), min.	199.69
Temperature range (K), max.	433.25

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.65213e+01
Coeff. B	-5.32656e+03
Coeff. C	-1.13601e+01
Coeff. D	1.63841e-05
Temperature range (K), min.	156.08
Temperature range (K), max.	433.25

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1260

Chemical Modeling of the TMA-CO2-H2O System: A Draw Solution in Forward Osmosis for Process Water Recovery: https://www.doi.org/10.1021/acs.jced.6b00780

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=C75503&Units=SI

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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/mol1260.mol

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
gf:	Standard Gibbs free energy of formation
gyrad:	Radius of Gyration
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
svapt:	Entropy of vaporization at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility
zra:	Rackett Parameter