Benzene, 1-methyl-3-nitro-

Other names:	1-Methyl-3-nitrobenzene
	3-Methyl-1-nitrobenzene
	3-Methylnitrobenzene
	3-NT
	3-NT (3-nitrotoluene)
	3-Nitrotoluene
	3-Nitrotoluol
	MNT
	Toluene, m-nitro-
	UN 1664
	m-Methylnitrobenzene
	m-Nitrotoluene
	m-mononitrotoluene
	toluene, 3-nitro-
Inchi:	InChI=1S/C7H7NO2/c1-6-3-2-4-7(5-6)8(9)10/h2-5H,1H3
InchiKey:	QZYHIOPPLUPUJF-UHFFFAOYSA-N
Formula:	C7H7NO2
SMILES:	Cc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	137.14
CAS:	99-08-1

Physical Properties

Property code	Value	Unit	Source
chl	-3723.50 ± 3.30	kJ/mol	NIST Webbook
chl	-3737.00	kJ/mol	NIST Webbook
chl	-3721.90	kJ/mol	NIST Webbook
ea	0.80 ± 0.10	eV	NIST Webbook
ea	1.18 ± 0.05	eV	NIST Webbook
ea	0.93	eV	NIST Webbook
ea	0.97 ± 0.03	eV	NIST Webbook
ea	0.98 ± 0.05	eV	NIST Webbook
ea	0.99 ± 0.10	eV	NIST Webbook
gf	146.39	kJ/mol	Joback Method
hf	26.49	kJ/mol	Joback Method
hfl	-46.00	kJ/mol	NIST Webbook
hfus	18.90	kJ/mol	Joback Method
hvap	50.70	kJ/mol	Joback Method

ie	9.50 ± 0.10	eV	NIST Webbook
ie	9.50 ± 0.10	eV	NIST Webbook
ie	9.48	eV	NIST Webbook
ie	9.65 ± 0.05	eV	NIST Webbook
ie	9.50 ± 0.10	eV	NIST Webbook
ie	9.50	eV	NIST Webbook
ie	9.49 ± 0.01	eV	NIST Webbook
log10ws	-2.45		Aqueous Solubility Prediction Method
log10ws	-2.44		Estimated Solubility Method
logp	1.903		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
nfpah	%!d(float64=2)		KDB
nfpas	%!d(float64=4)		KDB
pc	4098.62	kPa	Joback Method
rinpol	1201.00		NIST Webbook
rinpol	202.07		NIST Webbook
rinpol	1201.00		NIST Webbook
tb	505.75	K	KDB
tb	504.00 ± 0.40	K	NIST Webbook
tb	503.70	K	NIST Webbook
tb	505.80	K	NIST Webbook
tb	503.95 ± 0.40	K	NIST Webbook
tc	793.00	K	Joback Method
tf	289.00 ± 2.00	K	NIST Webbook
tf	288.59 ± 0.20	K	NIST Webbook
tf	289.20	K	KDB
tf	288.90	K	Aqueous Solubility Prediction Method
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.85	J/mol×K	626.37	Joback Method
cpg	232.54	J/mol×K	584.72	Joback Method
cpg	269.27	J/mol×K	751.34	Joback Method
cpg	261.18	J/mol×K	709.68	Joback Method
cpg	252.39	J/mol×K	668.03	Joback Method
cpg	221.40	J/mol×K	543.06	Joback Method

cpg	276.69	J/mol×K	793.00	Joback Method
cpl	202.10	J/mol×K	302.40	NIST Webbook
hfust	19.20	kJ/mol	370.00	NIST Webbook
hvapt	49.80	kJ/mol	429.00	NIST Webbook
hvapt	52.80	kJ/mol	424.50	NIST Webbook
hvapt	56.60 ± 2.50	kJ/mol	303.00	NIST Webbook
psub	3.39e-03	kPa	283.15	Gas Saturation Vapor Pressure Measurements of Mononitrotoluene Isomers from (283.15 to 313.15) K
pvap	0.07	kPa	323.10	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.03	kPa	308.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.03	kPa	308.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.04	kPa	313.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods

pvap	0.04	kPa	313.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	0.04	kPa	313.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	0.05	kPa	318.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	0.05	kPa	318.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	0.05	kPa	318.10	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	

pvap	0.03	kPa	308.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	0.07	kPa	323.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	0.07	kPa	323.10	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	0.10	kPa	328.10	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	0.03	kPa	308.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	

pvap	0.19	kPa	338.00	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	6.48e-03	kPa	290.60	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	8.42e-03	kPa	293.30	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	0.01	kPa	296.30	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	0.01	kPa	299.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	

pvap	0.02	kPa	302.30	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	0.02	kPa	305.30	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	0.03	kPa	308.30	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	0.03	kPa	311.40	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	0.04	kPa	314.30	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	

pvap	0.05	kPa	317.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	0.06	kPa	320.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	0.02	kPa	303.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	0.02	kPa	303.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	0.02	kPa	303.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	

pvap	0.02	kPa	302.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	0.01	kPa	299.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	0.07	kPa	323.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	0.14	kPa	333.10	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	0.01	kPa	298.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	

rhol	1147.67	kg/m3	303.15	Effect of various substituents on benzene ring and their impact on volumetric, acoustic and transport properties of binary liquid mixtures with dimethylacetamide	
rhol	1137.98	kg/m3	313.15	Thermodynamics of binary mixtures: The effect of substituents in aromatics on their excess properties with benzylalcohol	
rhol	1142.67	kg/m3	308.15	Thermodynamics of binary mixtures: The effect of substituents in aromatics on their excess properties with benzylalcohol	
rhol	1147.67	kg/m3	303.15	Thermodynamics of binary mixtures: The effect of substituents in aromatics on their excess properties with benzylalcohol	
rhol	1152.23	kg/m3	298.15	Thermodynamics of binary mixtures: The effect of substituents in aromatics on their excess properties with benzylalcohol	
rhol	1147.62	kg/m3	303.15	Excess Volumes, Speeds of Sound, Isentropic Compressibilities, and Viscosities of Binary Mixtures of Acetophenone with Chlorotoluenes and Nitrotoluenes at 303.15 K	

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.62065e+01
Coeff. B	-5.73455e+03
Coeff. C	-8.83600e+00
Temperature range (K), min.	369.07
Temperature range (K), max.	535.18

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.85531e+00
Coeff. B	-5.34312e+03
Coeff. C	2.04059e+00
Coeff. D	-1.50181e-06
Temperature range (K), min.	289.20
Temperature range (K), max.	734.00

Datasets

Viscosity, Pa*s

Pressure, kPa - Liquid	Temperature, K - Liquid	Viscosity, Pa*s - Liquid
101.00	303.15	0.0017770

Reference *https://www.doi.org/10.1016/j.jct.2006.04.005*

Sources

Assessing the Salting-Out Behavior of Nitrobenzene, 2-Nitrotoluene, and 3-Nitrotoluene from Solubility Values in Pure Water and Seawater at Temperatures between (277 and 314) K: https://www.doi.org/10.1021/je800624c

Thermodynamics of binary mixtures:	https://www.doi.org/10.1016/j.fluid.2014.01.019
The effect of substituents in aromatics on their excess properties with benzylalcohol:	http://link.springer.com/article/10.1007/BF02311772
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
Densities and ultrasonic studies for binary mixtures of tetrahydrofuran with chlorobenzenes, chlorotoluenes and nitrotoluenes at 298.15 K:	https://www.doi.org/10.1016/j.fluid.2011.07.018
Benchmark properties of 2-, 3-, and 4-nitrotoluene. Evaluation of thermochemical data with complementary experimental and computational methods:	https://www.doi.org/10.1016/j.jct.2017.03.029
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Effect of various substituents on benzene ring and their impact on volumetric, acoustic and transport properties of binary liquid mixtures with dimethylacetamide:	https://www.doi.org/10.1016/j.fluid.2015.03.048
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C99081&Units=SI
Excess Volumes, Speeds of Sound, Isentropic Compressibilities, and Viscosities of Binary Mixtures of Acetophenone with Chlorotoluenes and Nitrotoluenes at 303.15 K:	https://www.doi.org/10.1021/je050413l
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1451
Gas Saturation Vapor Pressure Measurements of Mononitrotoluene Isomers from (283.15 to 313.15) K:	https://www.doi.org/10.1021/je900293j
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1451
Volumetric, ultrasonic and viscometric studies of binary mixtures of dimethyl sulphoxide with chloro and nitro substituted aromatic hydrocarbons at T = 303.15 K:	https://www.doi.org/10.1016/j.jct.2006.04.005

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
nfpas:	NFPA Safety Rating
pc:	Critical Pressure
psub:	Sublimation pressure
pvap:	Vapor pressure

rhol:	Liquid Density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume