Benzene, 1-methyl-2-nitro-

Other names:	1-Methyl-2-Nitrobenzene
	2-Methyl-1-nitrobenzene
	2-Methylnitrobenzene
	2-NT
	2-NT (2-nitrotoluene)
	2-Nitrotoluene
	NSC 9577
	ONT
	Toluene, o-nitro-
	o-Methylnitrobenzene
	o-Nitrotoluene
	o-mononitrotoluene
Inchi:	InChI=1S/C7H7NO2/c1-6-4-2-3-5-7(6)8(9)10/h2-5H,1H3
InchiKey:	PLAZTCDQAHEYBI-UHFFFAOYSA-N
Formula:	C7H7NO2
SMILES:	Cc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	137.14
CAS:	88-72-2

Physical Properties

Property code	Value	Unit	Source
chl	-3745.30 ± 3.80	kJ/mol	NIST Webbook
chl	-3754.00	kJ/mol	NIST Webbook
ea	0.92 ± 0.10	eV	NIST Webbook
ea	0.95 ± 0.05	eV	NIST Webbook
ea	0.88 ± 0.03	eV	NIST Webbook
ea	1.24 ± 0.05	eV	NIST Webbook
gf	146.39	kJ/mol	Joback Method
hf	26.49	kJ/mol	Joback Method
hfus	18.90	kJ/mol	Joback Method
hvap	59.10 ± 0.30	kJ/mol	NIST Webbook
hvap	59.60 ± 1.60	kJ/mol	NIST Webbook
ie	9.69 ± 0.01	eV	NIST Webbook
ie	9.63	eV	NIST Webbook
ie	9.50	eV	NIST Webbook
ie	9.51 ± 0.03	eV	NIST Webbook
ie	9.24	eV	NIST Webbook

ie	9.24	eV	NIST Webbook
ie	10.20 ± 0.10	eV	NIST Webbook
ie	9.43 ± 0.05	eV	NIST Webbook
log10ws	-2.32		Aqueous Solubility Prediction Method
log10ws	-2.33		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	194.65		NIST Webbook
rinpol	194.65		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1155.00		NIST Webbook
ripol	1877.00		NIST Webbook
ripol	1877.00		NIST Webbook
tb	495.00 ± 0.30	K	NIST Webbook
tb	494.85	K	KDB
tb	495.45 ± 0.50	K	NIST Webbook
tb	495.30 ± 0.07	K	NIST Webbook
tb	494.90	K	NIST Webbook
tb	498.20	K	NIST Webbook
tb	495.45 ± 0.40	K	NIST Webbook
tb	498.85 ± 1.00	K	NIST Webbook
tc	793.00	K	Joback Method
tf	270.05 ± 0.30	K	NIST Webbook
tf	269.98	K	KDB
tf	270.25 ± 0.20	K	NIST Webbook
tf	269.06 ± 0.05	K	NIST Webbook
tf	282.60 ± 0.50	K	NIST Webbook
tf	263.60 ± 0.30	K	NIST Webbook
tf	269.30 ± 0.30	K	NIST Webbook
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.40	J/mol×K	543.06	Joback Method
cpg	242.85	J/mol×K	626.37	Joback Method

cpg	252.39	J/mol×K	668.03	Joback Method
cpg	261.18	J/mol×K	709.68	Joback Method
cpg	269.27	J/mol×K	751.34	Joback Method
cpg	276.69	J/mol×K	793.00	Joback Method
cpg	232.54	J/mol×K	584.72	Joback Method
cpl	202.50	J/mol×K	302.30	NIST Webbook
hvapt	59.00 ± 0.30	kJ/mol	298.50	NIST Webbook
hvapt	52.00	kJ/mol	418.00	NIST Webbook
hvapt	51.00	kJ/mol	449.00	NIST Webbook
hvapt	52.20	kJ/mol	440.00	NIST Webbook
pvap	5.26e-03	kPa	283.30	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.02	kPa	298.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.02	kPa	298.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.03	kPa	303.10	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods

pvap	3.20e-03	kPa	278.40	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.04	kPa	308.10	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.04	kPa	308.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.06	kPa	313.10	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.01	kPa	293.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods

pvap	0.08	kPa	318.00	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.08	kPa	318.10	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.11	kPa	323.00	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	5.53e-03	kPa	283.15	Gas Saturation Vapor Pressure Measurements of Mononitrotoluene Isomers from (283.15 to 313.15) K
pvap	0.01	kPa	293.15	Gas Saturation Vapor Pressure Measurements of Mononitrotoluene Isomers from (283.15 to 313.15) K
pvap	0.03	kPa	303.15	Gas Saturation Vapor Pressure Measurements of Mononitrotoluene Isomers from (283.15 to 313.15) K
pvap	0.06	kPa	313.15	Gas Saturation Vapor Pressure Measurements of Mononitrotoluene Isomers from (283.15 to 313.15) K

pvap	0.01	kPa	293.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	8.04e-03	kPa	288.30	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	8.06e-03	kPa	288.30	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	5.02e-03	kPa	283.30	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.03	kPa	303.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods

pvap	0.06	kPa	313.10	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	
pvap	3.28e-03	kPa	278.30	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods	
rhol	1153.24	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	1144.91	kg/m3	313.15	Thermodynamics of binary mixtures: The effect of substituents in aromatics on their excess properties with benzylalcohol	
rhol	1149.78	kg/m3	308.15	Thermodynamics of binary mixtures: The effect of substituents in aromatics on their excess properties with benzylalcohol	
rhol	1153.29	kg/m3	303.15	Thermodynamics of binary mixtures: The effect of substituents in aromatics on their excess properties with benzylalcohol	

rhol	1159.60	kg/m3	298.15	Thermodynamics of binary mixtures: The effect of substituents in aromatics on their excess properties with benzylalcohol
rhol	1153.26	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	1.40926e+01
Coeff. B	-3.45189e+03
Coeff. C	-1.31655e+02
Temperature range (K), min.	381.70
Temperature range (K), max.	524.76

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	4.91453e+01
Coeff. B	-7.84782e+03
Coeff. C	-4.67886e+00
Coeff. D	1.48976e-06
Temperature range (K), min.	269.98
Temperature range (K), max.	720.00

Datasets

Viscosity, Pa*s

Pressure, kPa - Liquid	Temperature, K - Liquid	Viscosity, Pa*s - Liquid
101.00	303.15	0.0019110
Reference		*https://www.doi.org/10.1016/j.jct.2006.04.005*

Sources

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=C88722&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Thermodynamics of binary mixtures: The effect of substituents in aromatics on their excess properties with benzylalcohol.:	https://www.doi.org/10.1016/j.fluid.2014.01.019
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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1450
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
Volumetric, ultrasonic and viscometric studies of binary mixtures of dimethyl [illegible] substituted aromatic hydrocarbons at T = 303.15 K:	https://www.doi.org/10.1016/j.jct.2006.04.005
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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
Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermodynamic data with complementary experimental and computational methods:	https://www.doi.org/10.1016/j.jct.2017.03.029
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1450
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
Solubility of Imidazoles, Benzimidazoles, and Phenylimidazoles in Dichloromethane, 1-Chlorobutane, Toluene, and 2-Nitrotoluene:	https://www.doi.org/10.1021/je049907t
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Gas Saturation Vapor Pressure Measurements of Mononitrotoluene Isomers from (283.15 to 313.15) K:	https://www.doi.org/10.1021/je900293j

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
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
nfpas:	NFPA Safety Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
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