

# Benzene, 1-methyl-4-nitro-

<b>Other names:</b>	1-Methyl-4-nitrobenzene 4-Methylnitrobenzene 4-NT 4-NT (4-nitrotoluene) 4-Nitrotoluene 4-Nitrotoluol 4-methyl-1-nitrobenzene NCI-C60537 NSC 9579 PNT Toluene, p-nitro- p-Methylnitrobenzene p-Nitrotoluene para-nitrotoluene toluene, 4-nitro-
<b>Inchi:</b>	InChI=1S/C7H7NO2/c1-6-2-4-7(5-3-6)8(9)10/h2-5H,1H3
<b>InchiKey:</b>	ZPTVNYMJQHSSEA-UHFFFAOYSA-N
<b>Formula:</b>	C7H7NO2
<b>SMILES:</b>	Cc1ccc([N+](=O)[O-])cc1
<b>Mol. weight [g/mol]:</b>	137.14
<b>CAS:</b>	99-99-0

## Physical Properties

Property code	Value	Unit	Source
affp	815.20	kJ/mol	NIST Webbook
basg	782.70	kJ/mol	NIST Webbook
chs	-3719.00	kJ/mol	NIST Webbook
chs	-3706.90 ± 2.90	kJ/mol	NIST Webbook
ea	0.96 ± 0.03	eV	NIST Webbook
ea	1.10 ± 0.05	eV	NIST Webbook
ea	0.95 ± 0.10	eV	NIST Webbook
ea	0.97 ± 0.05	eV	NIST Webbook
ea	0.93 ± 0.09	eV	NIST Webbook
gf	146.39	kJ/mol	Joback Method
hf	30.90 ± 3.90	kJ/mol	NIST Webbook
hfs	-48.20 ± 3.00	kJ/mol	NIST Webbook
hfus	18.90	kJ/mol	Joback Method

hsub	74.80 ± 1.00	kJ/mol	NIST Webbook
hsub	79.10 ± 2.50	kJ/mol	NIST Webbook
hsub	79.10	kJ/mol	NIST Webbook
hsub	79.00 ± 3.00	kJ/mol	NIST Webbook
hvap	50.70	kJ/mol	Joback Method
ie	9.56	eV	NIST Webbook
ie	9.54 ± 0.01	eV	NIST Webbook
ie	9.52	eV	NIST Webbook
ie	9.50 ± 0.10	eV	NIST Webbook
ie	9.76 ± 0.05	eV	NIST Webbook
ie	9.10 ± 0.10	eV	NIST Webbook
ie	9.46 ± 0.05	eV	NIST Webbook
ie	9.46 ± 0.05	eV	NIST Webbook
log10ws	-2.49		Aqueous Solubility Prediction Method
log10ws	-2.49		Estimated Solubility Method
logp	1.903		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
nfpah	%!d(float64=1)		KDB
nfpas	%!d(float64=3)		KDB
pc	4098.62	kPa	Joback Method
rinpol	1170.00		NIST Webbook
rinpol	1212.00		NIST Webbook
rinpol	1195.00		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	205.47		NIST Webbook
ripol	1986.00		NIST Webbook
tb	511.49	K	KDB
tc	793.00	K	Joback Method
tf	325.47	K	Aqueous Solubility Prediction Method
tf	324.75	K	KDB
tt	324.78 ± 0.00	K	NIST Webbook
vc	0.402	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.69	J/mol×K	793.00	Joback Method
cpg	232.54	J/mol×K	584.72	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	221.40	J/mol×K	543.06	Joback Method
cps	172.30	J/mol×K	298.15	NIST Webbook
hfust	16.81	kJ/mol	324.80	NIST Webbook
hfust	16.81	kJ/mol	324.80	NIST Webbook
hfust	16.90	kJ/mol	318.00	NIST Webbook
hvapt	54.20	kJ/mol	440.00	NIST Webbook
hvapt	49.80	kJ/mol	467.50	NIST Webbook
hvapt	52.80	kJ/mol	432.00	NIST Webbook
psub	0.03	kPa	321.15	Triacetone tr Peroxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	0.02	kPa	315.15	Triacetone tr Peroxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	0.03	kPa	319.15	Triacetone tr Peroxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	0.01	kPa	311.15	Triacetone tr Peroxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	1.25e-03	kPa	283.15	Gas Saturation Vapor Pressure Measurements of Mononitrotoluene Isomers from (283.15 to 313.15) K

p <sub>sub</sub>	3.79e-03	kPa	293.15	Gas Saturation Vapor Pressure Measurements of Mononitrotoluene Isomers from (283.15 to 313.15) K
p <sub>sub</sub>	0.01	kPa	303.15	Gas Saturation Vapor Pressure Measurements of Mononitrotoluene Isomers from (283.15 to 313.15) K
p <sub>sub</sub>	0.03	kPa	313.15	Gas Saturation Vapor Pressure Measurements of Mononitrotoluene Isomers from (283.15 to 313.15) K
p <sub>sub</sub>	7.96e-03	kPa	307.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
p <sub>sub</sub>	5.11e-03	kPa	303.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
p <sub>vap</sub>	0.12	kPa	333.00	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
p <sub>vap</sub>	0.09	kPa	328.10	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods

pvap	0.09	kPa	328.10	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.34	kPa	350.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.11	kPa	333.00	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.16	kPa	338.00	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.15	kPa	338.00	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods

pvap	0.22	kPa	343.00	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.21	kPa	343.00	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.27	kPa	347.90	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.29	kPa	348.00	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.37	kPa	352.90	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods

pvap	0.37	kPa	353.00	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.48	kPa	357.90	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.50	kPa	358.00	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.62	kPa	362.90	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.66	kPa	363.00	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods

pvap	0.84	kPa	367.90	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.79	kPa	367.90	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.08	kPa	326.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.10	kPa	329.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.12	kPa	332.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods

pvap	0.12	kPa	332.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.14	kPa	335.30	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.17	kPa	338.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.20	kPa	341.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.24	kPa	344.40	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods

pvap	0.28	kPa	347.10	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.40	kPa	353.20	Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of thermochemical data with complementary experimental and computational methods
sfust	53.10	J/mol×K	318.00	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.66992e+01
Coeff. B	-6.27318e+03
Coeff. C	8.26700e+00
Temperature range (K), min.	373.97
Temperature range (K), max.	542.61

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	1.62314e+01
Coeff. B	-5.95994e+03
Coeff. C	-6.57033e-03
Coeff. D	2.79656e-07
Temperature range (K), min.	324.75
Temperature range (K), max.	736.00

# Sources

<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C99990&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C99990&amp;Units=SI</a>
<b>KDB Vapor Pressure Data:</b>	<a href="https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1452">https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1452</a>
<b>Benchmark properties of 2-, 3- and 4-nitrotoluene: Evaluation of McGowan's method</b>	<a href="https://www.doi.org/10.1016/j.jct.2017.03.029">https://www.doi.org/10.1016/j.jct.2017.03.029</a>
<b>Determination of Mononitrotoluene, 2,6-Dinitrotoluene, 2,3-Dinitrotoluene, 2,4-Dinitrotoluene, 2,5-Dinitrotoluene, 2,6,4-Trinitrotoluene in Pure Water by Gas Chromatographic Method: A Thermogravimetric study of vapor pressure and enthalpy of sublimation in 303–338 K temperature range: Gas Saturation Vapor Pressure Measurements of Mononitrotoluene Estimated Solubility Method (9.15) K:</b>	<a href="https://www.doi.org/10.1016/j.tca.2010.11.034">https://www.doi.org/10.1016/j.tca.2010.11.034</a>
<b>KDB:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Aqueous Solubility Prediction Method:</b>	<a href="https://www.doi.org/10.1021/je900293j">https://www.doi.org/10.1021/je900293j</a>
<b>Joback Method:</b>	<a href="http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt">http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt</a>
	<a href="https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1452">https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1452</a>
	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

## Legend

<b>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity
<b>chs:</b>	Standard solid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>cps:</b>	Solid phase heat capacity
<b>ea:</b>	Electron affinity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfs:</b>	Solid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>nfpaf:</b>	NFPA Fire Rating
<b>nfpah:</b>	NFPA Health Rating
<b>nfpas:</b>	NFPA Safety Rating

<b>pc:</b>	Critical Pressure
<b>psub:</b>	Sublimation pressure
<b>pvap:</b>	Vapor pressure
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>sfust:</b>	Entropy of fusion at a given temperature
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>tt:</b>	Triple Point Temperature
<b>vc:</b>	Critical Volume

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