Benzene, 1-methyl-4-nitro-

Other names:	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-
Inchi:	InChI=1S/C7H7NO2/c1-6-2-4-7(5-3-6)8(9)10/h2-5H,1H3
InchiKey:	ZPTVNYMJQHSSEA-UHFFFAOYSA-N
Formula:	C7H7NO2
SMILES:	Cc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	137.14
CAS:	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	-3706.90 ± 2.90	kJ/mol	NIST Webbook
chs	-3719.00	kJ/mol	NIST Webbook
ea	0.96 ± 0.03	eV	NIST Webbook
ea	1.10 ± 0.05	eV	NIST Webbook
ea	0.97 ± 0.05	eV	NIST Webbook
ea	0.95 ± 0.10	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	79.00 ± 3.00	kJ/mol	NIST Webbook
hsub	79.10	kJ/mol	NIST Webbook
hvap	50.70	kJ/mol	Joback Method
ie	9.46 ± 0.05	eV	NIST Webbook
ie	9.52	eV	NIST Webbook
ie	9.50 ± 0.10	eV	NIST Webbook
ie	9.10 ± 0.10	eV	NIST Webbook
ie	9.56	eV	NIST Webbook
ie	9.76 ± 0.05	eV	NIST Webbook
ie	9.54 ± 0.01	eV	NIST Webbook
ie	9.46 ± 0.05	eV	NIST Webbook
log10ws	-2.49		Estimated Solubility Method
log10ws	-2.49		Aqueous Solubility Prediction 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	1167.00		NIST Webbook
rinpol	205.47		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1212.00		NIST Webbook
rinpol	1195.00		NIST Webbook
ripol	1986.00		NIST Webbook
tb	511.49	K	KDB
tc	793.00	K	Joback Method
tf	324.75	K	KDB
tf	325.47	K	Aqueous Solubility Prediction Method
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	269.27	J/mol×K	751.34	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	276.69	J/mol×K	793.00	Joback Method
cpg	232.54	J/mol×K	584.72	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	52.80	kJ/mol	432.00	NIST Webbook
hvapt	49.80	kJ/mol	467.50	NIST Webbook
hvapt	54.20	kJ/mol	440.00	NIST Webbook
psub	5.11e-03	kPa	303.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	0.03	kPa	313.15	Gas Saturation Vapor Pressure Measurements of Mononitrotoluene Isomers from (283.15 to 313.15) K
psub	0.01	kPa	303.15	Gas Saturation Vapor Pressure Measurements of Mononitrotoluene Isomers from (283.15 to 313.15) K
psub	3.79e-03	kPa	293.15	Gas Saturation Vapor Pressure Measurements of Mononitrotoluene Isomers from (283.15 to 313.15) K
psub	0.03	kPa	321.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range

psub	0.03	kPa	319.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range	
psub	0.02	kPa	315.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range	
psub	0.01	kPa	311.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range	
psub	7.96e-03	kPa	307.15	Triacetone triperoxide 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	
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	0.16	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	0.11	kPa	333.00	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	0.12	kPa	333.00	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	0.40	kPa	353.20	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	0.09	kPa	328.10	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
sfust	53.10	J/mol×K	318.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = 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(Pvp) = 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

Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range:	https://www.doi.org/10.1016/j.tca.2010.11.034
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1452
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1452
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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C99990&Units=SI
Solubility of 4-Nitrotoluene, 2,6-Dinitrotoluene, 2,3-Dinitrotoluene, and 1,3,5-Trinitrobenzene in Pure Water and Seawater:	https://www.doi.org/10.1021/je700374j
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Gas Saturation Vapor Pressure Measurements of Mononitrotoluene Isomers from (283.15 to 313.15) K:	https://www.doi.org/10.1021/je900293j

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
psub:	Sublimation pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume