

1,2,4-Trimethylbenzene

Other names:	1,2,4-trimethylbenzene (pseudocumene) 1,2,5-Trimethylbenzene 1,3,4-Trimethylbenzene AS-TRIMETHYBENZENE Asymmetrical trimethylbenzene Benzene, 1,2,5-trimethyl- NSC 65600 Pseudocumol Psi-cumene as-Trimethylbenzene benzene, 1,2,4-trimethyl- pseudocumene «psi»-Cumene
Inchi:	InChI=1S/C9H12/c1-7-4-5-8(2)9(3)6-7/h4-6H,1-3H3
InchiKey:	GWHJZXIDMPWGK-UHFFFAOYSA-N
Formula:	C9H12
SMILES:	Cc1ccc(C)c(C)c1
Mol. weight [g/mol]:	120.19
CAS:	95-36-3

Physical Properties

Property code	Value	Unit	Source
af	0.3760		KDB
cpl	213.02	J/mol×K	Thermodynamics of mixtures involving some (benzene derivatives + benzonitrile)
gf	117.00	kJ/mol	KDB
hcg	5194.77	kJ/mol	KDB
hcn	4930.677	kJ/mol	KDB
hf	-13.94	kJ/mol	KDB
hfus	12.33	kJ/mol	Joback Method
hvap	49.57	kJ/mol	Cheméo Relay (1.0)
ie	8.14	eV	Cheméo Relay (1.0)
log10ws	-3.31		Estimated Solubility Method
log10ws	-3.31		Aqueous Solubility Prediction Method

logp	2.612		Crippen Method
mcvol	113.910	ml/mol	McGowan Method
pc	3232.00	kPa	KDB
pc	3230.00 ± 40.00	kPa	NIST Webbook
tb	442.53	K	KDB
tb	442.45	K	Isobaric (vapour + liquid) equilibria for N-formylmorpholine with ethylbenzene, n-butylbenzene, iso-propylbenzene and 1,2,4-trimethylbenzene at 101.33 kPa
tc	649.10 ± 0.50	K	NIST Webbook
tc	649.10	K	KDB
tf	229.30	K	KDB
tf	229.25	K	Aqueous Solubility Prediction Method
vc	0.435	m3/kmol	KDB
zc	0.2605030		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.86	J/mol×K	616.95	Joback Method
cpg	216.81	J/mol×K	441.96	Joback Method
cpg	229.86	J/mol×K	476.96	Joback Method
cpg	242.27	J/mol×K	511.96	Joback Method
cpg	254.06	J/mol×K	546.96	Joback Method
cpg	265.25	J/mol×K	581.96	Joback Method
cpg	285.90	J/mol×K	651.95	Joback Method
dvisc	0.0002083	Pa×s	441.96	Joback Method
dvisc	0.0003221	Pa×s	375.52	Joback Method
dvisc	0.0009182	Pa×s	275.87	Joback Method
dvisc	0.0006008	Pa×s	309.09	Joback Method
dvisc	0.0004268	Pa×s	342.31	Joback Method
dvisc	0.0015760	Pa×s	242.65	Joback Method
dvisc	0.0002545	Pa×s	408.74	Joback Method
hvapt	39.25	kJ/mol	442.30	KDB
pvap	39.80	kPa	408.87	Phase equilibria on five binary systems containing 1-butanethiol and 3-methylthiophene in hydrocarbons

pvap	30.30	kPa	400.11	Phase equilibria on five binary systems containing 1-butanethiol and 3-methylthiophene in hydrocarbons
pvap	101.40	kPa	442.22	Phase equilibria on five binary systems containing 1-butanethiol and 3-methylthiophene in hydrocarbons
pvap	90.40	kPa	437.83	Phase equilibria on five binary systems containing 1-butanethiol and 3-methylthiophene in hydrocarbons
pvap	80.30	kPa	433.42	Phase equilibria on five binary systems containing 1-butanethiol and 3-methylthiophene in hydrocarbons
pvap	70.30	kPa	428.53	Phase equilibria on five binary systems containing 1-butanethiol and 3-methylthiophene in hydrocarbons
pvap	60.00	kPa	422.84	Phase equilibria on five binary systems containing 1-butanethiol and 3-methylthiophene in hydrocarbons
pvap	50.30	kPa	416.75	Phase equilibria on five binary systems containing 1-butanethiol and 3-methylthiophene in hydrocarbons
pvap	16.90	kPa	383.15	Phase equilibria on five binary systems containing 1-butanethiol and 3-methylthiophene in hydrocarbons
pvap	20.10	kPa	387.74	Phase equilibria on five binary systems containing 1-butanethiol and 3-methylthiophene in hydrocarbons

pvap	0.73	kPa	313.15	Vapor-liquid equilibria and excess enthalpies of the binary systems 1-pentanol or 2-pentanol and 1-hexene or 1,2,4-trimethylbenzene for the development of biofuels
rfi	1.50470		293.15	Isobaric Vapor Liquid Equilibrium Data for the System of 1-Methyl-2-Ethylbenzene + 1,2,4-Trimethylbenzene at 10 kPa
rfi	1.50237		298.15	KDB
rhof	875.78	kg/m3	293.15	Isobaric VLE data for 1-methyl-3-ethylbenzene or 1-methyl-4-ethylbenzene + 1,2,4-trimethylbenzene at 20 kPa
rhof	871.64	kg/m3	298.15	Excess Molar volumes and Surface Tensions of Trimethylbenzene with Tetrahydrofuran Tetrachloromethane and Dimethylsulfoxide at 298.15 K
rhof	871.64	kg/m3	298.15	Excess Molar Volumes and Surface Tensions of 1,2,4-Trimethylbenzene and 1,3,5-Trimethylbenzene with 1-Butanol, 2-Methyl-1-propanol, 2-Butanol, and 2-Methyl-2-propanol at 298.15 K
rhof	880.00	kg/m3	289.00	KDB
srf	0.03	N/m	298.15	Excess Molar Volumes and Surface Tensions of Trimethylbenzene + Ethylene Glycol Ester at 298.15 K and 313.15 K
srf	0.03	N/m	293.20	KDB

srf	0.03	N/m	313.15	Excess Molar Volumes and Surface Tensions of 1,2,4-Trimethylbenzene and 1,3,5-Trimethylbenzene with Isopropyl Acetate and Isobutyl Acetate at (298.15, 308.15, and 313.15) K
srf	0.03	N/m	308.15	Excess Molar Volumes and Surface Tensions of 1,2,4-Trimethylbenzene and 1,3,5-Trimethylbenzene with Isopropyl Acetate and Isobutyl Acetate at (298.15, 308.15, and 313.15) K
srf	0.03	N/m	298.15	Excess Molar Volumes and Surface Tensions of 1,2,4-Trimethylbenzene and 1,3,5-Trimethylbenzene with Isopropyl Acetate and Isobutyl Acetate at (298.15, 308.15, and 313.15) K
srf	0.03	N/m	313.15	Excess Molar Volumes and Surface Tensions of 1,2,4-Trimethylbenzene and 1,3,5-Trimethylbenzene with 1,1-Diethoxyethane and 2,2-Dimethoxypropane at (298.15, 308.15, and 313.15) K

srf	0.03	N/m	313.15	Excess Molar Volumes and Surface Tensions of 1,2,4-Trimethylbenzene and 1,3,5-Trimethylbenzene with 1,1-Diethoxyethane and 2,2-Dimethoxypropane at (298.15, 308.15, and 313.15) K
srf	0.03	N/m	308.15	Excess Molar Volumes and Surface Tensions of 1,2,4-Trimethylbenzene and 1,3,5-Trimethylbenzene with 1,1-Diethoxyethane and 2,2-Dimethoxypropane at (298.15, 308.15, and 313.15) K
srf	0.03	N/m	298.15	Excess Molar Volumes and Surface Tensions of 1,2,4-Trimethylbenzene and 1,3,5-Trimethylbenzene with 1,1-Diethoxyethane and 2,2-Dimethoxypropane at (298.15, 308.15, and 313.15) K
srf	0.03	N/m	313.15	Densities and Surface Tensions of Trimethylbenzene + Dimethyl Carbonate or + Diethyl Carbonate at 298.15 K and 313.15 K
srf	0.03	N/m	298.15	Densities and Surface Tensions of Trimethylbenzene + Dimethyl Carbonate or + Diethyl Carbonate at 298.15 K and 313.15 K

srf	0.03	N/m	313.15	Excess Molar Volumes and Surface Tensions of Trimethylbenzene + Ethylene Glycol Ester at 298.15 K and 313.15 K
srf	0.03	N/m	313.15	Densities, surface tensions, and derived surface thermodynamics properties of (trimethylbenzene + propyl acetate, or butyl acetate) from T = 298.15 K to 313.15 K
srf	0.03	N/m	308.15	Densities, surface tensions, and derived surface thermodynamics properties of (trimethylbenzene + propyl acetate, or butyl acetate) from T = 298.15 K to 313.15 K
srf	0.03	N/m	303.15	Densities, surface tensions, and derived surface thermodynamics properties of (trimethylbenzene + propyl acetate, or butyl acetate) from T = 298.15 K to 313.15 K
srf	0.03	N/m	298.15	Densities, surface tensions, and derived surface thermodynamics properties of (trimethylbenzene + propyl acetate, or butyl acetate) from T = 298.15 K to 313.15 K
tcondl	0.13	W/m×K	257.79	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl	0.13	W/m×K	295.54	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	257.93	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	276.33	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	276.54	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	276.69	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl	0.13	W/m×K	283.32	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	283.54	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	283.68	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	257.58	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	295.76	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl	0.13	W/m×K	295.91	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	312.75	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	312.98	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	313.13	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	330.69	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl	0.12	W/m×K	330.93	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	331.09	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.47784e+01
Coeff. B	-4.06027e+03
Coeff. C	-4.29020e+01
Temperature range (K), min.	323.10
Temperature range (K), max.	471.79

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	6.15931e+01
Coeff. B	-7.42775e+03
Coeff. C	-6.69353e+00
Coeff. D	2.96938e-06
Temperature range (K), min.	229.38
Temperature range (K), max.	649.13

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
273.15	100.00	891.7
273.15	1000.00	892.3
273.15	2000.00	892.9
273.15	5000.00	894.6
273.15	10000.00	897.4
273.15	15000.00	900.2
273.15	20000.00	902.8
273.15	30000.00	908.0
273.15	40000.00	912.9
273.15	50000.00	917.5
273.15	60000.00	921.9
273.15	70000.00	926.2
273.15	80000.00	930.3
273.15	90000.00	934.2
273.15	100000.00	938.0
273.15	110000.00	941.7
273.15	120000.00	945.2
273.15	130000.00	948.6
273.15	140000.00	952.0
283.15	100.00	883.3
283.15	1000.00	883.9
283.15	2000.00	884.5
283.15	5000.00	886.3
283.15	10000.00	889.3
283.15	15000.00	892.2
283.15	20000.00	895.0
283.15	30000.00	900.3
283.15	40000.00	905.4
283.15	50000.00	910.2
283.15	60000.00	914.8
283.15	70000.00	919.3
283.15	80000.00	923.5
283.15	90000.00	927.5
283.15	100000.00	931.4
283.15	110000.00	935.2

283.15	120000.00	938.9
283.15	130000.00	942.4
283.15	140000.00	945.8
293.15	100.00	875.1
293.15	1000.00	875.7
293.15	2000.00	876.3
293.15	5000.00	878.2
293.15	10000.00	881.4
293.15	15000.00	884.4
293.15	20000.00	887.3
293.15	30000.00	892.9
293.15	40000.00	898.2
293.15	50000.00	903.2
293.15	60000.00	908.0
293.15	70000.00	912.6
293.15	80000.00	916.9
293.15	90000.00	921.1
293.15	100000.00	925.1
293.15	110000.00	929.0
293.15	120000.00	932.8
293.15	130000.00	936.4
293.15	140000.00	939.9
303.15	100.00	867.0
303.15	1000.00	867.6
303.15	2000.00	868.3
303.15	5000.00	870.3
303.15	10000.00	873.6
303.15	15000.00	876.8
303.15	20000.00	879.8
303.15	30000.00	885.7
303.15	40000.00	891.2
303.15	50000.00	896.4
303.15	60000.00	901.4
303.15	70000.00	906.1
303.15	80000.00	910.6
303.15	90000.00	914.9
303.15	100000.00	919.1
303.15	110000.00	923.1
303.15	120000.00	927.0
303.15	130000.00	930.7
303.15	140000.00	934.3
313.15	100.00	859.0
313.15	1000.00	859.7
313.15	2000.00	860.4

313.15	5000.00	862.6
313.15	10000.00	866.0
313.15	15000.00	869.3
313.15	20000.00	872.6
313.15	30000.00	878.7
313.15	40000.00	884.5
313.15	50000.00	889.9
313.15	60000.00	895.0
313.15	70000.00	899.9
313.15	80000.00	904.6
313.15	90000.00	909.0
313.15	100000.00	913.3
313.15	110000.00	917.4
313.15	120000.00	921.4
313.15	130000.00	925.2
313.15	140000.00	928.9
323.15	100.00	851.3
323.15	1000.00	852.0
323.15	2000.00	852.7
323.15	5000.00	855.0
323.15	10000.00	858.6
323.15	15000.00	862.1
323.15	20000.00	865.5
323.15	30000.00	871.9
323.15	40000.00	877.9
323.15	50000.00	883.5
323.15	60000.00	888.9
323.15	70000.00	894.0
323.15	80000.00	898.8
323.15	90000.00	903.4
323.15	100000.00	907.8
323.15	110000.00	912.0
323.15	120000.00	916.1
323.15	130000.00	920.0
323.15	140000.00	923.8
333.15	100.00	843.6
333.15	1000.00	844.4
333.15	2000.00	845.2
333.15	5000.00	847.6
333.15	10000.00	851.4
333.15	15000.00	855.1
333.15	20000.00	858.6
333.15	30000.00	865.3
333.15	40000.00	871.6

333.15	50000.00	877.4
333.15	60000.00	883.0
333.15	70000.00	888.2
333.15	80000.00	893.2
333.15	90000.00	898.0
333.15	100000.00	902.5
333.15	110000.00	906.9
333.15	120000.00	911.1
333.15	130000.00	915.1
333.15	140000.00	919.0

Reference

<https://www.doi.org/10.1016/j.jct.2017.03.006>

Viscosity, Pa*s

Temperature, K - Liquid	Pressure, kPa - Liquid	Viscosity, Pa*s - Liquid
293.15	100.00	0.0008929
293.15	1000.00	0.0009065
293.15	5000.00	0.0009417
293.15	10000.00	0.0009769
293.15	20000.00	0.0010610
293.15	30000.00	0.0011479
293.15	40000.00	0.0012332
293.15	50000.00	0.0013362
293.15	60000.00	0.0014349
293.15	70000.00	0.0015664
293.15	80000.00	0.0016926
293.15	100000.00	0.0019518
293.15	120000.00	0.0022875
293.15	140000.00	0.0026681
313.15	100.00	0.0006989
313.15	1000.00	0.0007096
313.15	5000.00	0.0007359
313.15	10000.00	0.0007606
313.15	20000.00	0.0008203
313.15	30000.00	0.0008894
313.15	40000.00	0.0009528
313.15	50000.00	0.0010264
313.15	60000.00	0.0010996
313.15	70000.00	0.0011708
313.15	80000.00	0.0012493

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=663
Thermophysical properties of 1,2,4-trimethylbenzene in admixtures with 1-butanol at accurate high pressure piecewise measurements: Vibrating wire viscometer and falling body viscometer techniques:	https://www.doi.org/10.1016/j.jct.2017.03.006
Isobaric (vapour + liquid) equilibria for N-formylmorpholine with ethylbenzene, Methylbenzene, iso-propylbenzene and 1,2,4-trimethylbenzene at 101.33 kPa: Excess Molar Volumes and Surface Tensions of 1,2,4-Trimethylbenzene and 1,2,4-trimethylbenzene binary systems containing 2-Methoxyethanol, 2-Propanol, and 1,2-Methyl-2-propanol Data for the System of	https://www.doi.org/10.1016/j.jct.2015.12.021
SMALL 1,2-Ethylbenzene + 1-methyl-2-ethylbenzene at 10 kPa: Modified Acetylene Density approach for determination of vaporization and Excess Molar Volumes and Surface Tensions of 1,2,4-Trimethylbenzene and 1,2,4-trimethylbenzene binary systems at 298.15 K and 313.15 K:	https://en.wikipedia.org/wiki/Joback_method
Viscosities of binary mixtures containing 1-butanol + 2,2,4-trimethylpentane): + 1,2,4-trimethylbenzene at high pressures for the thermophysical characterization of biofuels:	https://www.doi.org/10.1016/j.jct.2012.04.016
Solubilities at High Dilution of Toluene, Ethylbenzene, 1,2,4-Trimethylbenzene, and Hexane in 2-Pentanone, 1,1,1-Trichloroethane, and 2,2,2-Trifluoroethane:	http://link.springer.com/article/10.1007/BF02311772
Determination of Partitioning Coefficients of Numerous Organics Sources and their Aqueous Solubility as a Function of Temperature:	https://www.doi.org/10.1021/je049807n
1,2,4-trimethylbenzene for the development of biofuels	https://www.doi.org/10.1016/j.fluid.2010.02.030
Carbonic acid equilibria in carbonate systems with 1,2,4-trimethylbenzene and water + 2,2,4-trimethylbenzene and water + derived surface thermodynamic parameters for 1,2,4-trimethylbenzene + propyl acetate, or butyl acetate) from T = 298.15 K to 313.15 K:	https://www.doi.org/10.1021/je301122r
Excess Molar Volumes and Surface Tensions of 1,2,4- Trimethylbenzene and 1,2,4-trimethylbenzene with 1,2,4-trimethylbenzene and 1,2,4-trimethylbenzene results, isopropyl acetate and isobutyl acetate at (298.15, 308.15, and 313.15) K:	https://www.doi.org/10.1016/j.jct.2013.01.016

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hcg:	Heat of Combustion, Gross form
hcn:	Heat of Combustion, Net Form
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
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhol:	Liquid Density
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tcondl:	Liquid thermal conductivity
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility

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