Benzene, (1-methylethyl)-

Other names:	(1-METHYLETHYL)BENZENE
	(1-methylethyl)benzene (cumene)
	(Methylethyl)benzene
	1-methylethylbenzene
	2-Fenilpropano
	2-Fenyl-propaan
	2-PHENYLPROPANE
	Benzene, i-propyl-
	Benzene, isopropyl-
	Cumeen
	Cumene
	Cumol
	ISOPROPYLBENZENE
	Isopropilbenzene
	Isopropylbenzeen
	Isopropylbenzol
	NSC 8776
	Propane, 2-phenyl-
	Rcra waste number U055
	UN 1918
	i-Propylbenzene
	iso-propylbenzene
	iso-propylbenzene (cumene)
Inchi:	InChI=1S/C9H12/c1-8(2)9-6-4-3-5-7-9/h3-8H,1-2H3
InchiKey:	RWGFKTVRMDUZSP-UHFFFAOYSA-N
Formula:	C9H12
SMILES:	CC(C)c1ccccc1
Mol. weight [g/mol]:	120.19
CAS:	98-82-8

Physical Properties

Property code	Value	Unit	Source
af	0.3260		KDB
affp	791.60	kJ/mol	NIST Webbook
aigt	698.15	K	KDB
basg	763.90	kJ/mol	NIST Webbook

chl	-5215.44 ± 0.96	kJ/mol	NIST Webbook
chl	-5218.60	kJ/mol	NIST Webbook
cpl	214.75	J/mol×K	Thermodynamics of mixtures involving some (benzene derivatives + benzonitrile)
dvisc	0.0007390	Pa×s	Viscosities, Densities, and Speeds of Sound of Binary Mixtures of o-Xylene, m-Xylene, p-Xylene, and Isopropylbenzene with 2-Butanone at 298.15 K
dvisc	0.0007390	Pa×s	Viscosities, Densities, and Speeds of Sound of Binary Mixtures of o-Xylene, m-Xylene, p-Xylene, and Isopropylbenzene with 4-Methylpentan-2-one at 298.15 K
fll	0.90	% in Air	KDB
flu	6.50	% in Air	KDB
fpo	317.04	K	KDB
gf	137.10	kJ/mol	KDB
hcg	5215.44	kJ/mol	KDB
hcn	4951.346	kJ/mol	KDB
hf	3.90 ± 1.10	kJ/mol	NIST Webbook
hf	3.94	kJ/mol	KDB
hfl	-41.20 ± 1.10	kJ/mol	NIST Webbook
hfus	9.58	kJ/mol	Joback Method
hvap	44.00	kJ/mol	NIST Webbook
hvap	45.15	kJ/mol	NIST Webbook
hvap	45.10	kJ/mol	NIST Webbook
hvap	45.10	kJ/mol	NIST Webbook
hvap	45.14	kJ/mol	NIST Webbook
hvap	45.10	kJ/mol	NIST Webbook
hvap	37.00	kJ/mol	NIST Webbook
hvap	45.10	kJ/mol	NIST Webbook
hvap	45.10 ± 0.10	kJ/mol	NIST Webbook
ie	8.98	eV	NIST Webbook
ie	8.76	eV	NIST Webbook
ie	8.71	eV	NIST Webbook
ie	8.73 ± 0.02	eV	NIST Webbook
ie	8.72 ± 0.01	eV	NIST Webbook
ie	8.69 ± 0.01	eV	NIST Webbook
ie	8.75	eV	NIST Webbook
ie	8.72	eV	NIST Webbook
log10ws	-3.27		Aqueous Solubility Prediction Method
log10ws	-3.27		Estimated Solubility Method

logp	2.810		Crippen Method
mcvol	113.910	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
pc	3209.00 ± 6.00	kPa	NIST Webbook
pc	3210.00 ± 40.00	kPa	NIST Webbook
pc	2786.44 ± 151.99	kPa	NIST Webbook
pc	3209.00	kPa	KDB
pc	3160.00 ± 5.88	kPa	NIST Webbook
rhoc	278.84 ± 0.96	kg/m3	NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	911.30		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	904.10		NIST Webbook
rinpol	906.70		NIST Webbook
rinpol	920.40		NIST Webbook
rinpol	925.60		NIST Webbook
rinpol	931.80		NIST Webbook
rinpol	915.50		NIST Webbook
rinpol	900.30		NIST Webbook
rinpol	907.00		NIST Webbook
rinpol	903.40		NIST Webbook
rinpol	903.90		NIST Webbook
rinpol	904.10		NIST Webbook
rinpol	904.10		NIST Webbook
rinpol	906.70		NIST Webbook
rinpol	908.00		NIST Webbook
rinpol	939.00		NIST Webbook
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rinpol	930.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	935.00		NIST Webbook

rinpol	937.00	NIST Webbook
rinpol	940.00	NIST Webbook
rinpol	910.10	NIST Webbook
rinpol	910.10	NIST Webbook
rinpol	910.10	NIST Webbook
rinpol	910.10	NIST Webbook
rinpol	910.10	NIST Webbook
rinpol	910.10	NIST Webbook
rinpol	908.00	NIST Webbook
rinpol	905.00	NIST Webbook
rinpol	908.00	NIST Webbook
rinpol	911.00	NIST Webbook
rinpol	913.00	NIST Webbook
rinpol	916.00	NIST Webbook
rinpol	915.00	NIST Webbook
rinpol	903.10	NIST Webbook
rinpol	910.80	NIST Webbook
rinpol	903.50	NIST Webbook
rinpol	932.00	NIST Webbook
rinpol	940.00	NIST Webbook
rinpol	947.00	NIST Webbook
rinpol	924.00	NIST Webbook
rinpol	909.00	NIST Webbook
rinpol	915.00	NIST Webbook
rinpol	932.00	NIST Webbook
rinpol	925.10	NIST Webbook
rinpol	917.00	NIST Webbook
rinpol	909.00	NIST Webbook
rinpol	927.00	NIST Webbook
rinpol	911.00	NIST Webbook
rinpol	912.20	NIST Webbook
rinpol	912.00	NIST Webbook
rinpol	910.00	NIST Webbook
rinpol	927.00	NIST Webbook
rinpol	914.30	NIST Webbook
rinpol	919.40	NIST Webbook
rinpol	922.20	NIST Webbook
rinpol	923.60	NIST Webbook
rinpol	906.90	NIST Webbook
rinpol	930.30	NIST Webbook
rinpol	929.00	NIST Webbook
rinpol	926.00	NIST Webbook
rinpol	910.80	NIST Webbook
rinpol	928.70	NIST Webbook

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rinpol	910.00	NIST Webbook
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rinpol	926.00	NIST Webbook
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rinpol	907.00	NIST Webbook
rinpol	916.00	NIST Webbook
rinpol	922.00	NIST Webbook
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rinpol	920.10	NIST Webbook

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rinpol	942.50	NIST Webbook
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rinpol	909.82	NIST Webbook
rinpol	909.10	NIST Webbook
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ripol	1169.80	NIST Webbook
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ripol	1236.00	NIST Webbook
ripol	1198.00	NIST Webbook
ripol	1205.00	NIST Webbook
ripol	1213.00	NIST Webbook
ripol	1191.00	NIST Webbook
ripol	1161.00	NIST Webbook
ripol	1182.00	NIST Webbook
ripol	1192.30	NIST Webbook
ripol	1177.00	NIST Webbook
ripol	1181.00	NIST Webbook
ripol	1166.00	NIST Webbook
ripol	1186.00	NIST Webbook
ripol	1189.00	NIST Webbook
ripol	1200.00	NIST Webbook
ripol	1211.00	NIST Webbook
ripol	1225.00	NIST Webbook
ripol	1169.00	NIST Webbook
ripol	1179.00	NIST Webbook
ripol	1155.00	NIST Webbook
ripol	1168.00	NIST Webbook
ripol	1185.00	NIST Webbook

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ripol	1182.00		NIST Webbook
ripol	1177.00		NIST Webbook
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ripol	1164.00		NIST Webbook
ripol	1161.00		NIST Webbook
ripol	1162.00		NIST Webbook
ripol	1186.00		NIST Webbook
ripol	1158.00		NIST Webbook
sg	386.53	J/mol×K	NIST Webbook
sl	277.57	J/mol×K	NIST Webbook
tb	425.63	K	Experimental Isobaric Vapor-Liquid Equilibrium Data for Binary Mixtures of Cyclic Ethers with (1-Methylethyl)benzene
tb	425.44	K	Vapor-Liquid Equilibrium Data for N-Methylacetamide and N,N-Dimethylacetamide with Cumene at 97.3 kPa
tb	425.55	K	Isobaric (vapour + liquid) equilibria for N-formylmorpholine with ethylbenzene, n-butylbenzene, iso-propylbenzene and 1,2,4-trimethylbenzene at 101.33 kPa
tb	425.55	K	Isobaric (vapour + liquid) equilibria for sulfolane with toluene, ethylbenzene, and isopropylbenzene at 101.33 kPa
tb	425.56	K	KDB
tb	425.44	K	Isobaric Vapor Liquid Equilibrium of Binary Mixtures of Vinyl Acetate and Ethyl Formate with Cumene at 97.3 kPa
tc	635.90 ± 4.00	K	NIST Webbook
tc	631.00	K	KDB
tc	631.00 ± 0.50	K	NIST Webbook
tc	631.10 ± 0.15	K	NIST Webbook
tc	624.55 ± 2.00	K	NIST Webbook
tf	177.14	K	KDB
tt	177.13 ± 0.01	K	NIST Webbook

vc	0.435	m3/kmol	KDB
zc	0.2658850		KDB
zra	0.26		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.92	J/mol×K	573.00	Joback Method
cpg	279.29	J/mol×K	608.35	Joback Method
cpg	214.82	J/mol×K	431.56	Joback Method
cpg	229.30	J/mol×K	466.92	Joback Method
cpg	242.96	J/mol×K	502.28	Joback Method
cpg	255.82	J/mol×K	537.64	Joback Method
cpg	289.96	J/mol×K	643.71	Joback Method
cpl	214.40	J/mol×K	295.96	NIST Webbook
cpl	198.70	J/mol×K	302.00	NIST Webbook
cpl	215.40	J/mol×K	298.15	NIST Webbook
cpl	209.41	J/mol×K	299.80	NIST Webbook
cpl	213.00	J/mol×K	298.00	NIST Webbook
cpl	198.70	J/mol×K	302.00	NIST Webbook
dvisc	0.0006110	Pa×s	313.15	Density and Viscosity of Propyl Formate + Aromatic Hydrocarbons at T = (303.15, 308.15, and 313.15) K
dvisc	0.0006110	Pa×s	313.15	Physical Properties of Binary Mixtures of Ethyl Formate with Benzene, Isopropyl Benzene, Isobutyl Benzene, and Butylbenzene at (303.15, 308.15, and 313.15) K

dvisc	0.0006510	Pa×s	308.15	Physical Properties of Binary Mixtures of Ethyl Formate with Benzene, Isopropyl Benzene, Isobutyl Benzene, and Butylbenzene at (303.15, 308.15, and 313.15) K	
dvisc	0.0006900	Pa×s	303.15	Physical Properties of Binary Mixtures of Ethyl Formate with Benzene, Isopropyl Benzene, Isobutyl Benzene, and Butylbenzene at (303.15, 308.15, and 313.15) K	
dvisc	0.0006510	Pa×s	308.15	Density and Viscosity of Propyl Formate + Aromatic Hydrocarbons at T = (303.15, 308.15, and 313.15) K	
dvisc	0.0006900	Pa×s	303.15	Density and Viscosity of Propyl Formate + Aromatic Hydrocarbons at T = (303.15, 308.15, and 313.15) K	
hfust	7.33	kJ/mol	177.13	NIST Webbook	
hfust	7.32	kJ/mol	177.10	NIST Webbook	
hfust	7.32	kJ/mol	177.10	NIST Webbook	
hvapt	41.90	kJ/mol	384.50	NIST Webbook	
hvapt	41.20	kJ/mol	387.50	NIST Webbook	
hvapt	42.10	kJ/mol	386.00	NIST Webbook	
rfi	1.49130		293.15	Liquid liquid equilibria of ternary systems (water + carboxylic acid + cumene) at 298.15K	
rfi	1.48869		298.15	Effect of Temperature on the Change of Refractive Index on Mixing for Butyl Acetate + Aromatic Hydrocarbons	

rfi	1.48890		298.15	KDB
rfi	1.49005		298.20	Salt Effects on Liquid-Liquid Equilibria of Water + Phenol + (Propan-2-yl) Benzene + Salts Systems
rfi	1.49120		293.15	Experimental and correlational study of phase equilibria in aqueous mixtures of phosphoric acid with aromatic hydrocarbons at various temperatures
rhol	864.12	kg/m3	298.15	Liquid-Liquid Equilibrium for Ternary Systems, Water + 5-Hydroxymethylfurfural + (1-Butanol, Isobutanol, Methyl Isobutyl Ketone), at 313.15, 323.15, and 333.15 K
rhol	862.00	kg/m3	293.00	KDB
rhol	857.51	kg/m3	298.15	Thermodynamic study of 1,1,2,2-tetrachloroethane + hydrocarbon mixtures I. Excess and solvation enthalpies
rhol	857.54	kg/m3	298.20	Liquid-Liquid Equilibrium of the Ternary System of Water + Phenol + (Propan-2-yl) Benzene at Several Temperatures
sfust	41.37	J/mol×K	177.10	NIST Webbook
sfust	41.36	J/mol×K	177.13	NIST Webbook
srf	0.03	N/m	293.20	KDB

tcondl	0.11	W/m×K	329.45	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.12	W/m×K	294.11	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.12	W/m×K	275.40	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.12	W/m×K	275.24	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.12	W/m×K	275.03	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	

tcondl	0.13	W/m×K	261.48	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.13	W/m×K	261.33	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.13	W/m×K	261.13	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.12	W/m×K	294.32	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.12	W/m×K	312.46	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	

tcondl	0.12	W/m×K	312.68	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.12	W/m×K	312.84	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.11	W/m×K	329.83	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.11	W/m×K	329.68	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.12	W/m×K	294.47	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(Pvp) = A + B/(T + C)
Coeff. A	1.43493e+01
Coeff. B	-3.63341e+03
Coeff. C	-5.21730e+01
Temperature range (K), min.	310.56
Temperature range (K), max.	454.20

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.02480e+02
Coeff. B	-8.96989e+03
Coeff. C	-1.29151e+01
Coeff. D	7.67090e-06
Temperature range (K), min.	177.14
Temperature range (K), max.	631.15

Datasets

Speed of sound, m/s

Temperature, K - Liquid	Pressure, kPa - Liquid	Speed of sound, m/s - Liquid
298.15	100.00	1309.1
313.15	100.00	1247.6
333.15	100.00	1168.5
353.15	100.00	1091.8
373.15	100.00	1017.8
393.15	100.00	945.6
413.15	100.00	875.0
433.15	10100.00	897.7
298.15	20100.00	1406.9

313.15	20100.00	1351.3
333.15	20100.00	1280.5
353.15	20100.00	1213.2
373.15	20100.00	1149.2
393.15	20100.00	1088.1
413.15	20100.00	1029.6
433.15	20100.00	974.0
298.15	40100.00	1491.7
313.15	40100.00	1440.0
333.15	40100.00	1374.7
353.15	40100.00	1313.2
373.15	40100.00	1255.1
393.15	40100.00	1200.1
413.15	40100.00	1147.8
433.15	40100.00	1098.9
298.15	60100.00	1566.8
313.15	60100.00	1518.3
333.15	60100.00	1457.2
353.15	60100.00	1399.6
373.15	60100.00	1345.6
393.15	60100.00	1294.7
413.15	60100.00	1246.5
433.15	60100.00	1201.3
298.15	80100.00	1634.8
313.15	80100.00	1588.9
333.15	80100.00	1530.9
353.15	80100.00	1476.5
373.15	80100.00	1425.6
393.15	80100.00	1377.6
413.15	80100.00	1332.1
433.15	80100.00	1289.9
298.15	100100.00	1697.4
313.15	100100.00	1653.3
333.15	100100.00	1598.0
353.15	100100.00	1546.0
373.15	100100.00	1497.4
393.15	100100.00	1451.6
413.15	100100.00	1408.6
433.15	100100.00	1368.6

Reference *https://www.doi.org/10.1016/j.jct.2019.03.005*

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
298.15	100.00	857.94
313.15	100.00	845.05
333.15	100.00	827.73
353.15	100.00	810.17
373.15	100.00	792.31
393.15	100.00	773.98
413.15	100.00	755.04
433.15	10100.00	752.29
298.15	20100.00	871.79
313.15	20100.00	859.97
333.15	20100.00	844.44
353.15	20100.00	828.86
373.15	20100.00	813.36
393.15	20100.00	797.74
413.15	20100.00	781.98
433.15	20100.00	766.12
298.15	40100.00	883.81
313.15	40100.00	872.84
333.15	40100.00	858.51
353.15	40100.00	844.27
373.15	40100.00	830.23
393.15	40100.00	816.2
413.15	40100.00	802.25
433.15	40100.00	788.34
298.15	60100.00	894.47
313.15	60100.00	884.19
333.15	60100.00	870.78
353.15	60100.00	857.52
373.15	60100.00	844.51
393.15	60100.00	831.6
413.15	60100.00	818.85
433.15	60100.00	806.14
298.15	80100.00	904.16
313.15	80100.00	894.38
333.15	80100.00	881.68
353.15	80100.00	869.22
373.15	80100.00	857.0
393.15	80100.00	844.92
413.15	80100.00	833.04

433.15	80100.00	821.27
298.15	100100.00	913.02
313.15	100100.00	903.69
333.15	100100.00	891.56
353.15	100100.00	879.74
373.15	100100.00	868.11
393.15	100100.00	856.72
413.15	100100.00	845.53
433.15	100100.00	834.45

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Legend

af:	Acentric Factor
affp:	Proton affinity
aigt:	Autoignition Temperature
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
fll:	Lower Flammability Limit
flu:	Upper Flammability Limit
fpo:	Flash Point (Open Cup Method)
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
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
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sg:	Molar entropy at standard conditions
sl:	Liquid phase molar entropy at standard conditions
speedsl:	Speed of sound in fluid
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tcondl:	Liquid thermal conductivity
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility
zra:	Rackett Parameter