

1-Butanol, 3-methyl-

Other names:	2-Methyl-4-butanol
	3-Methyl-1-butanol
	3-Methylbutan-1-ol
	3-Methylbutanol
	3-Metil-butanolo
	3-methylbutanol
	Alcool amilico
	Alcool isoamylique
	Amylowy alkohol
	Butan-1-ol, 3-methyl
	Butanol, 3-methyl-
	Fermentation amyl alcohol
	Fusel Oil
	ISOAMYL ALCOHOL
	ISOBUTYL CARBINOL
	ISOPENTYL ALCOHOL
	Isoamyl alcohol (3-methyl butanol)
	Isoamyl alcohol, primary
	Isoamylol
	Isopentan-1-ol
	Isopentanol
	Methyl-3-butan-1-ol
	NSC 1029
	i-Amyl alcohol
	iso-amylalkohol
Inchi:	InChI=1S/C5H12O/c1-5(2)3-4-6/h5-6H,3-4H2,1-2H3
InchiKey:	PHTQWCKDNZKARW-UHFFFAOYSA-N
Formula:	C5H12O
SMILES:	CC(C)CCO
Mol. weight [g/mol]:	88.15
CAS:	123-51-3

Physical Properties

Property code	Value	Unit	Source
chl	-3326.60 ± 1.60	kJ/mol	NIST Webbook
chl	-3326.20 ± 0.50	kJ/mol	NIST Webbook

dm	1.80	debye	KDB
gf	-148.04	kJ/mol	Joback Method
hf	-302.30	kJ/mol	KDB
hf	-300.80	kJ/mol	NIST Webbook
hf	-301.30 ± 1.50	kJ/mol	NIST Webbook
hfl	-355.90 ± 1.60	kJ/mol	NIST Webbook
hfl	-356.40 ± 0.59	kJ/mol	NIST Webbook
hfus	9.27	kJ/mol	Joback Method
hvap	43.02	kJ/mol	Joback Method
log10ws	-0.52		Aqueous Solubility Prediction Method
log10ws	-0.51		Estimated Solubility Method
logp	1.025		Crippen Method
mcvol	87.180	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=1)		KDB
pc	4559.63 ± 202.65	kPa	NIST Webbook
pc	3930.00 ± 40.00	kPa	NIST Webbook
pc	3930.00 ± 20.00	kPa	NIST Webbook
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ripol	1209.00		NIST Webbook
ripol	1180.00		NIST Webbook
ripol	1200.00		NIST Webbook
tb	404.20	K	KDB
tb	404.50	K	Phase equilibria of (water + levunilic acid + alcohol) ternary systems
tb	404.90	K	Vapor liquid equilibrium of the ethanol + 3-methyl-1-butanol system at 50.66, 101.33 and 151.99 kPa
tb	404.55	K	(Liquid + liquid) equilibria of (water + butyric acid + isoamyl alcohol) ternary system
tb	404.45	K	Effect of Pressure on the Azeotrope of the Mixture Isoamyl Acetate Isoamyl Alcohol at 50.00, 101.32, 250.00, and 350.00 kPa

tb	404.27	K	Vapor-Liquid Equilibria at 101.3 kPa for Binary Mixtures Containing 2-Methyl-1-propanol + 2-Methyl-1-butanol, 2-Methyl-1-propanol + 3-Methyl-1-butanol, and 2-Methyl-1-propanol + 1-Pentanol
tc	577.20	K	KDB
tf	156.08	K	Aqueous Solubility Prediction Method
tf	155.90	K	KDB
tt	118.00	K	Heat Capacities in the Solid and in the Liquid Phase of Isomeric Pentanols
vc	0.329	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.20 ± 1.10	J/mol×K	451.65	NIST Webbook
cpg	193.70 ± 1.10	J/mol×K	474.55	NIST Webbook
cpg	197.60 ± 1.10	J/mol×K	488.35	NIST Webbook
cpg	200.70 ± 1.10	J/mol×K	499.15	NIST Webbook
cpl	210.00	J/mol×K	303.00	NIST Webbook
cpl	209.52	J/mol×K	295.52	NIST Webbook
cpl	257.70	J/mol×K	347.00	NIST Webbook
dvisc	0.3005917	Pa×s	191.93	Joback Method
dvisc	0.0010745	Pa×s	334.34	Joback Method
dvisc	0.0026559	Pa×s	298.74	Joback Method
dvisc	0.0005174	Pa×s	369.94	Joback Method
dvisc	0.0002833	Pa×s	405.54	Joback Method
dvisc	0.0379452	Pa×s	227.53	Joback Method
dvisc	0.0083860	Pa×s	263.13	Joback Method
hvapt	57.10	kJ/mol	357.50	NIST Webbook
hvapt	54.20 ± 0.20	kJ/mol	313.00	NIST Webbook
hvapt	55.20 ± 0.20	kJ/mol	303.00	NIST Webbook
hvapt	51.40 ± 0.20	kJ/mol	343.00	NIST Webbook
hvapt	47.20	kJ/mol	355.00	NIST Webbook
hvapt	49.80	kJ/mol	376.00	NIST Webbook
hvapt	49.70 ± 0.20	kJ/mol	358.00	NIST Webbook
hvapt	44.07	kJ/mol	404.20	NIST Webbook
hvapt	56.50	kJ/mol	362.00	NIST Webbook

hvapt	52.90 ± 0.20	kJ/mol	328.00	NIST Webbook
kvisc	0.0000026	m2/s	318.15	Density, Viscosity, Excess Molar Volume, and Viscosity Deviation of Three Amyl Alcohols + Ethanol Binary Mixtures from 293.15 to 323.15 K
kvisc	0.0000023	m2/s	323.15	Density, Viscosity, Excess Molar Volume, and Viscosity Deviation of Three Amyl Alcohols + Ethanol Binary Mixtures from 293.15 to 323.15 K
kvisc	0.0000029	m2/s	313.15	Density, Viscosity, Excess Molar Volume, and Viscosity Deviation of Three Amyl Alcohols + Ethanol Binary Mixtures from 293.15 to 323.15 K
kvisc	0.0000033	m2/s	308.15	Density, Viscosity, Excess Molar Volume, and Viscosity Deviation of Three Amyl Alcohols + Ethanol Binary Mixtures from 293.15 to 323.15 K
kvisc	0.0000038	m2/s	303.15	Density, Viscosity, Excess Molar Volume, and Viscosity Deviation of Three Amyl Alcohols + Ethanol Binary Mixtures from 293.15 to 323.15 K

kvisc	0.0000044	m2/s	298.15	Density, Viscosity, Excess Molar Volume, and Viscosity Deviation of Three Amyl Alcohols + Ethanol Binary Mixtures from 293.15 to 323.15 K
kvisc	0.0000050	m2/s	293.15	Density, Viscosity, Excess Molar Volume, and Viscosity Deviation of Three Amyl Alcohols + Ethanol Binary Mixtures from 293.15 to 323.15 K
pvap	23.50	kPa	367.20	Complementary vapor pressure data for 2-methyl-1-propanol and 3-methyl-1-butanol at a pressure range of (15 to 177) kPa
pvap	91.50	kPa	402.00	Complementary vapor pressure data for 2-methyl-1-propanol and 3-methyl-1-butanol at a pressure range of (15 to 177) kPa
pvap	73.33	kPa	395.48	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2
pvap	108.50	kPa	407.00	Complementary vapor pressure data for 2-methyl-1-propanol and 3-methyl-1-butanol at a pressure range of (15 to 177) kPa
pvap	79.99	kPa	397.90	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2

pvap	86.66	kPa	400.18	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2
pvap	93.33	kPa	402.32	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2
pvap	97.99	kPa	403.77	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2
pvap	15.00	kPa	357.50	Complementary vapor pressure data for 2-methyl-1-propanol and 3-methyl-1-butanol at a pressure range of (15 to 177) kPa
pvap	32.00	kPa	374.40	Complementary vapor pressure data for 2-methyl-1-propanol and 3-methyl-1-butanol at a pressure range of (15 to 177) kPa
pvap	40.50	kPa	380.10	Complementary vapor pressure data for 2-methyl-1-propanol and 3-methyl-1-butanol at a pressure range of (15 to 177) kPa
pvap	61.33	kPa	390.64	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2
pvap	66.66	kPa	392.88	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2
pvap	55.99	kPa	388.23	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2

pvap	117.00	kPa	409.30	Complementary vapor pressure data for 2-methyl-1-propanol and 3-methyl-1-butanol at a pressure range of (15 to 177) kPa
pvap	50.66	kPa	385.62	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2
pvap	45.33	kPa	382.78	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2
pvap	40.00	kPa	379.65	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2
pvap	34.66	kPa	376.14	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2
pvap	30.66	kPa	373.24	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2
pvap	26.66	kPa	369.95	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2
pvap	176.50	kPa	422.40	Complementary vapor pressure data for 2-methyl-1-propanol and 3-methyl-1-butanol at a pressure range of (15 to 177) kPa
pvap	168.00	kPa	420.90	Complementary vapor pressure data for 2-methyl-1-propanol and 3-methyl-1-butanol at a pressure range of (15 to 177) kPa

pvap	159.50	kPa	419.20	Complementary vapor pressure data for 2-methyl-1-propanol and 3-methyl-1-butanol at a pressure range of (15 to 177) kPa
pvap	151.00	kPa	417.30	Complementary vapor pressure data for 2-methyl-1-propanol and 3-methyl-1-butanol at a pressure range of (15 to 177) kPa
pvap	142.50	kPa	415.40	Complementary vapor pressure data for 2-methyl-1-propanol and 3-methyl-1-butanol at a pressure range of (15 to 177) kPa
pvap	49.00	kPa	384.80	Complementary vapor pressure data for 2-methyl-1-propanol and 3-methyl-1-butanol at a pressure range of (15 to 177) kPa
pvap	134.00	kPa	413.50	Complementary vapor pressure data for 2-methyl-1-propanol and 3-methyl-1-butanol at a pressure range of (15 to 177) kPa
pvap	125.50	kPa	411.40	Complementary vapor pressure data for 2-methyl-1-propanol and 3-methyl-1-butanol at a pressure range of (15 to 177) kPa
pvap	22.66	kPa	366.27	Vapor pressure of selected aliphatic alcohols by ebulliometry. Part 2

pvap	66.00	kPa	392.80	Complementary vapor pressure data for 2-methyl-1-propanol and 3-methyl-1-butanol at a pressure range of (15 to 177) kPa
pvap	57.50	kPa	389.10	Complementary vapor pressure data for 2-methyl-1-propanol and 3-methyl-1-butanol at a pressure range of (15 to 177) kPa
rfi	1.40420		298.15	Isobaric Vapor Liquid Equilibrium for Binary and Ternary Systems of Isoamyl Alcohol + Isoamyl Acetate + Dimethyl Sulfoxide at 101.33 kPa
rfi	1.40530		298.15	Excess volumes and excess enthalpies of N-methyl-2-pyrrolidone with branched alcohols
rfi	1.40560		298.15	Physico-chemical and excess properties of the binary mixtures of methylcyclohexane + ethanol, + propan-1-ol, + propan-2-ol, + butan-1-ol, + 2-methyl-1-propanol, or 3-methyl-1-butanol at T = (298.15, 303.15, and 308.15) K

rfi	1.40340	303.15	Physico-chemical and excess properties of the binary mixtures of methylcyclohexane + ethanol, + propan-1-ol, + propan-2-ol, + butan-1-ol, + 2-methyl-1-propanol, or 3-methyl-1-butanol at T = (298.15, 303.15, and 308.15) K
rfi	1.40130	308.15	Physico-chemical and excess properties of the binary mixtures of methylcyclohexane + ethanol, + propan-1-ol, + propan-2-ol, + butan-1-ol, + 2-methyl-1-propanol, or 3-methyl-1-butanol at T = (298.15, 303.15, and 308.15) K
rfi	1.40500	298.15	Thermodynamic properties of (tetradecane + benzene, + toluene, + chlorobenzene, + bromobenzene, + anisole) binary mixtures at T = (298.15, 303.15, and 308.15) K
rfi	1.40100	308.15	Thermodynamic properties of (tetradecane + benzene, + toluene, + chlorobenzene, + bromobenzene, + anisole) binary mixtures at T = (298.15, 303.15, and 308.15) K

rfi	1.40500	298.15	Thermodynamic interactions in binary mixtures of anisole with ethanol, propan-1-ol, propan-2-ol, butan-1-ol, pentan-1-ol, and 3-methylbutan-1-ol at T = (298.15, 303.15, and 308.15) K
rfi	1.40300	303.15	Thermodynamic interactions in binary mixtures of anisole with ethanol, propan-1-ol, propan-2-ol, butan-1-ol, pentan-1-ol, and 3-methylbutan-1-ol at T = (298.15, 303.15, and 308.15) K
rfi	1.40350	303.15	Densities, Viscosities, Sound Speeds, Refractive Indices, and Excess Properties of Binary Mixtures of Isoamyl Alcohol with Some Alkoxyethanols
rfi	1.37820	308.15	Thermodynamic interactions in binary mixtures of anisole with ethanol, propan-1-ol, propan-2-ol, butan-1-ol, pentan-1-ol, and 3-methylbutan-1-ol at T = (298.15, 303.15, and 308.15) K
rfi	1.40530	298.15	Isobaric (vapour + liquid) equilibrium for N-methyl-2-pyrrolidone with branched alcohols

rfi	1.40850	298.20	Tie line data for the (water + butyric acid + n-butyl alcohol or amyl alcohol) at T = (298.2, 308.2, and 318.2) K and (water + butyric acid + isoamyl alcohol) at T = 298.2 K
rfi	1.40300	298.15	Experimental Binary VLE Data of Morpholine with 1-Butanol and 3-Methyl-1-butanol Systems
rfi	1.40540	293.15	Isobaric Vapor - Liquid Equilibria for the Ternary System of 2-Methyl-1-butanol, 3-Methyl-1-butanol, and Ethylene Glycol at 101.3 kPa
rfi	1.40515	298.15	Density, Refractive Index, Speed of Sound at 298.15 K, and Vapor-Liquid Equilibria at 101.3 kPa for Binary Mixtures of Propanol + 2-Methyl-1-butanol and Propanol + 3-Methyl-1-butanol
rfi	1.40510	298.15	Isobaric Vapor Liquid Equilibrium of 3-Methyl-1-butanol + Ethyl Lactate and 1-Pentanol + Ethyl Lactate at (13.0 and 101.3) kPa
rfi	1.41300	293.15	Liquid Liquid Equilibrium for the Ternary System 2-Methyl-1-propanol + 3-Methyl-1-butanol + Water at (298.15, 323.15, and 348.15) K

rfi	1.40470		298.15	Isobaric Vapor-Liquid Equilibria for Binary and Ternary Mixtures of Diisopropyl Ether, 2-Propyl Alcohol, and 3-Methyl-1-Butanol	
rfi	1.45010		298.15	Isobaric Vapor-Liquid Equilibrium for Binary Mixtures of 3-Methyl-1-butanol + 3-Methyl-1-butyl Ethanoate and 1-Pentanol + Pentyl Ethanoate at 101.3 kPa	
rfi	1.40300		303.15	Thermodynamic properties of (tetradecane + benzene, + toluene, + chlorobenzene, + bromobenzene, + anisole) binary mixtures at T = (298.15, 303.15, and 308.15) K	
rhoI	810.00	kg/m3	293.00	KDB	
rhoI	785.79	kg/m3	323.15	Volumetric and Viscometric Study of Binary Systems of Ethyl Butyrate with Alcohols	
rhoI	789.67	kg/m3	318.15	Volumetric and Viscometric Study of Binary Systems of Ethyl Butyrate with Alcohols	
rhoI	793.51	kg/m3	313.15	Volumetric and Viscometric Study of Binary Systems of Ethyl Butyrate with Alcohols	
rhoI	797.31	kg/m3	308.15	Volumetric and Viscometric Study of Binary Systems of Ethyl Butyrate with Alcohols	
rhoI	804.84	kg/m3	298.15	Volumetric and Viscometric Study of Binary Systems of Ethyl Butyrate with Alcohols	

rhoI	808.58	kg/m3	293.15	Volumetric and Viscometric Study of Binary Systems of Ethyl Butyrate with Alcohols
rhoI	812.29	kg/m3	288.15	Volumetric and Viscometric Study of Binary Systems of Ethyl Butyrate with Alcohols
rhoI	811.04	kg/m3	298.15	Isobaric Vapor Liquid Equilibria of Binary Systems (Propyl Acetate + n-Pentanol), (Propyl Acetate + 1-Methyl-1-butanol), and (Propyl Acetate + 3-Methyl-1-butanol) at 101.3 kPa
rhoI	806.21	kg/m3	298.15	Vapor Liquid Equilibrium of Mixtures Containing the Following Higher Alcohols: 2-Propanol, 2-Methyl-1-propanol, and 3-Methyl-1-butanol
rhoI	807.30	kg/m3	298.15	Isobaric Vapor Liquid Equilibrium for Two Binary Systems, (3-Methyl-1-butanol + 1,4-Butanediol) and (Hexylene Glycol + 1,4-Butanediol), at p = 40.0, 60.0, and 80.0 kPa
rhoI	796.95	kg/m3	308.15	Excess molar enthalpies of the binary systems: (Dibutyl ether + isomers of pentanol) at T = (298.15 and 308.15) K
rhoI	804.24	kg/m3	298.15	Excess molar enthalpies of the binary systems: (Dibutyl ether + isomers of pentanol) at T = (298.15 and 308.15) K

rhoI	794.43	kg/m3	313.20	Liquid-liquid equilibrium data and thermophysical properties for ternary systems composed of water, acetic acid and different solvents
rhoI	804.43	kg/m3	293.20	Liquid-liquid equilibrium data and thermophysical properties for ternary systems composed of water, acetic acid and different solvents
rhoI	808.94	kg/m3	298.20	Isothermal vapor-liquid equilibria, excess molar volume and the deviation of refractive indices for binary mixtures of 1-butanol, 1-hexanol, 3-methyl-1-butanol and butyl acetate
rhoI	807.16	kg/m3	298.20	Modeling phase equilibria of ternary systems (water + formic acid + ester or alcohol) through UNIFAC-original, SERLAS, NRTL, NRTL-modified, and three-suffix Margules: Parameter estimation using genetic algorithm
rhoI	778.14	kg/m3	332.70	Isothermal vapor liquid equilibria for different binary mixtures involved in the alcoholic distillation
rhoI	801.09	kg/m3	303.15	Volumetric and Viscometric Study of Binary Systems of Ethyl Butyrate with Alcohols

rhoI	803.20	kg/m3	303.15	Viscous synergy and antagonism and isentropic compressibility of ternary mixtures containing 1,3-dioxolane, water and monoalkanols at 303.15K
srf	0.02	N/m	323.15	Surface Tensions of Three Amyl Alcohol + Ethanol Binary Mixtures from (293.15 to 323.15) K
srf	0.02	N/m	318.15	Surface Tensions of Three Amyl Alcohol + Ethanol Binary Mixtures from (293.15 to 323.15) K
srf	0.02	N/m	313.15	Surface Tensions of Three Amyl Alcohol + Ethanol Binary Mixtures from (293.15 to 323.15) K
srf	0.02	N/m	308.15	Surface Tensions of Three Amyl Alcohol + Ethanol Binary Mixtures from (293.15 to 323.15) K
srf	0.02	N/m	303.15	Surface Tensions of Three Amyl Alcohol + Ethanol Binary Mixtures from (293.15 to 323.15) K
srf	0.02	N/m	293.15	Surface Tensions of Three Amyl Alcohol + Ethanol Binary Mixtures from (293.15 to 323.15) K
srf	0.02	N/m	328.15	Equilibrium surface tension and the interaction energy of DMSO with tert-butyl alcohol or iso-amyl alcohol at various temperatures

srf	0.02	N/m	318.15	Equilibrium surface tension and the interaction energy of DMSO with tert-butyl alcohol or iso-amyl alcohol at various temperatures
srf	0.02	N/m	308.15	Equilibrium surface tension and the interaction energy of DMSO with tert-butyl alcohol or iso-amyl alcohol at various temperatures
srf	0.02	N/m	298.15	Equilibrium surface tension and the interaction energy of DMSO with tert-butyl alcohol or iso-amyl alcohol at various temperatures
srf	0.02	N/m	298.15	Surface Tensions of Three Amyl Alcohol + Ethanol Binary Mixtures from (293.15 to 323.15) K

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.42576e+01
Coeff. B	-2.70339e+03
Coeff. C	-1.23544e+02
Temperature range (K), min.	317.06
Temperature range (K), max.	425.73

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$

Coeff. A	1.12297e+02
Coeff. B	-1.06664e+04
Coeff. C	-1.36325e+01
Coeff. D	3.26511e-06
Temperature range (K), min.	161.00
Temperature range (K), max.	579.45

Sources

Joback Method:

Separation of binary mixtures based on gamma infinity data using

Formanovic and Gaciv and

coefficients of infinite dilution functions:

Organic compounds in the non-liquid

of the Solvent:imidazolium chloride:

Isopropyl alcohol and methylimidazolium

butylmethylphosphonium hexafluorophosphate

Binary Mixtures of 1,3-Dioxane + 1-Butanol

Measurement and correlation of the

solubility of pentaerythritol in the

Effect of Pressure on the Solubility of

the Mixture Isoamyl Acetate Isoamyl

acetate + 2-methyl-2-butanol and

Binary Systems (Propyl Acetate +

Isopentanol or Propyl Acetate +

the ternary system of (Propyl

Acetate + methyl-1-butanol + 1-butanol,

aqueous vapor columns and the deviation

of the activity indices for binary mixtures

propyl alcohol + isopentanol ternary

mutual diffusion coefficients of

3-methyl-1-butanol and butyl acetate:

3-methyl-1-butanol + n-heptane and

Phase Equilibria in the Solid and the

liquid Phase of Isomeric Pentanols:

Liquid-liquid equilibrium data for water

+ formic acid + solvent (butyl acetate,

ethyl acetate, and isopentanol) at T

diffusion activity coefficients of propane,

propane liquid and isobutane, 1-butene,

isobutene, 1-butene, 2-butene, and

2-methyl-2-butene and correlation of

solubility of 2-methyl-2-butanol,

2-methyl-2-butanol (MNP) in ten pure

solvents from 283.15 K to 323.15 K:

The Yaws Handbook of Vapor

Pressure:

Solubilities of Hexadecanoic and

Octadecanoic Acids in Supercritical

CO₂ and vapor properties of

Co₂ and vapor properties of

(tetradecane + benzene, + toluene, +

solubility of benzene in isopentane +

isopentane + 1-butanol Solvent

solubility of benzene in isopentane +

solubility of benzene in isopentane +

solubility of benzene in isopentane +

solubility of benzene in isopentane +

solubility of benzene in isopentane +

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mcvol:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhof:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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