

Linalool

Other names:

(.+-.)-linalool
(.+/-.)-Linalool
1,6-Octadien-3-ol, 3,7-dimethyl-
2,6-Dimethyl-2,7-octadien-6-ol
2,6-Dimethyl-2,7-octadiene-6-ol
2,6-Dimethylocta-2,7-dien-6-ol
2,6-dimethyl-2,7-octadien-6-ol (linalool)
3,7-Dimethyl-1,6-octadien-3-ol
3,7-Dimethylocta-1,6-dien-3-ol
3,7-dimethyl-1,6-octadien-3-ol (linalool)
3,7-dimethyl-1,6-octandien-3-ol (linalool)
3,7-dimethylocta-1,6-dien-3-ol (linalool)
LINOLOOL (D)
Linalol
Linalool ex bois de rose oil
Linalool ex ho oil
Linalool ex orange oil
Linalool, «beta»
Linalool, Â«betaÂ»
Linaloyl oxide
Linalyl alcohol
Linanool
Linolool
NSC 3789
Phantol
allo-Ocimenol
b-Linalool
beta-Linalool
dl-2,6-dimethyl-2,7-octadien-6-ol
dl-3,7-Dimethyl-3-hydroxy-1,6-octadiene
dl-linalool
linalool B
p-Linalool
«beta»-Linalool
Â«betaÂ»-Linalool

Inchi: InChI=1S/C10H18O/c1-5-10(4,11)8-6-7-9(2)3/h5,7,11H,1,6,8H2,2-4H3

InchiKey: CDOSHBSSFJOMGT-UHFFFAOYSA-N

Formula: C10H18O

SMILES: C=CC(C)(O)CCC=C(C)C

Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
gf	58.85	kJ/mol	Joback Method
hf	-177.85	kJ/mol	Joback Method
hfus	15.94	kJ/mol	Joback Method
hvap	55.30	kJ/mol	NIST Webbook
hvap	65.00	kJ/mol	NIST Webbook
log10ws	-1.99		Estimated Solubility Method
log10ws	-1.99		Aqueous Solubility Prediction Method
logp	2.670		Crippen Method
mccvol	149.030	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
rinpol	1082.00		NIST Webbook
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ripol	1535.00	NIST Webbook
ripol	1507.00	NIST Webbook
ripol	1554.00	NIST Webbook
ripol	1537.00	NIST Webbook
ripol	1554.00	NIST Webbook
ripol	1507.00	NIST Webbook
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ripol	1533.00	NIST Webbook
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ripol	1547.00	NIST Webbook

ripol	1547.00	NIST Webbook
ripol	1521.00	NIST Webbook
ripol	1505.00	NIST Webbook
ripol	1550.00	NIST Webbook
ripol	1542.00	NIST Webbook
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ripol	1519.00	NIST Webbook
ripol	1540.00	NIST Webbook
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ripol	1507.00	NIST Webbook
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ripol	1574.00	NIST Webbook
ripol	1547.00	NIST Webbook
ripol	1547.00	NIST Webbook
ripol	1547.00	NIST Webbook
ripol	1537.00	NIST Webbook
ripol	1537.00	NIST Webbook
ripol	1542.00	NIST Webbook
ripol	1506.00	NIST Webbook
ripol	1506.00	NIST Webbook
ripol	1552.00	NIST Webbook
ripol	1537.00	NIST Webbook
ripol	1529.00	NIST Webbook
ripol	1500.00	NIST Webbook
ripol	1562.00	NIST Webbook
ripol	1544.00	NIST Webbook
ripol	1549.00	NIST Webbook
ripol	1547.00	NIST Webbook
ripol	1558.00	NIST Webbook
ripol	1539.00	NIST Webbook
ripol	1541.00	NIST Webbook
ripol	1569.00	NIST Webbook
ripol	1537.00	NIST Webbook

ripol	1566.00	NIST Webbook
ripol	1529.00	NIST Webbook
ripol	1553.00	NIST Webbook
ripol	1543.00	NIST Webbook
ripol	1525.00	NIST Webbook
ripol	1584.00	NIST Webbook
ripol	1526.00	NIST Webbook
ripol	1524.00	NIST Webbook
ripol	1558.00	NIST Webbook
ripol	1507.00	NIST Webbook
ripol	1544.00	NIST Webbook
ripol	1565.00	NIST Webbook
ripol	1543.00	NIST Webbook
ripol	1560.00	NIST Webbook
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ripol	1549.00	NIST Webbook
ripol	1534.00	NIST Webbook
ripol	1546.00	NIST Webbook
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ripol	1547.00	NIST Webbook
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ripol	1531.00	NIST Webbook
ripol	1540.00	NIST Webbook

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ripol	1508.00	NIST Webbook
ripol	1506.00	NIST Webbook
ripol	1513.00	NIST Webbook
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ripol	1506.00	NIST Webbook
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ripol	1535.00	NIST Webbook
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ripol	1537.00	NIST Webbook
ripol	1537.00	NIST Webbook
ripol	1537.00	NIST Webbook
ripol	1506.00	NIST Webbook
ripol	1552.00	NIST Webbook

ripol	1557.00		NIST Webbook
ripol	1558.00		NIST Webbook
ripol	1533.00		NIST Webbook
ripol	1558.00		NIST Webbook
ripol	1551.00		NIST Webbook
ripol	1552.00		NIST Webbook
ripol	1522.00		NIST Webbook
ripol	1498.00		NIST Webbook
ripol	1539.00		NIST Webbook
tb	471.80 ± 0.50	K	NIST Webbook
tb	471.80 ± 1.00	K	NIST Webbook
tb	471.80 ± 0.50	K	NIST Webbook
tb	471.75 ± 0.50	K	NIST Webbook
tc	697.57	K	Joback Method
tf	244.90	K	Joback Method
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.03	J/mol×K	517.87	Joback Method
cpg	360.38	J/mol×K	547.82	Joback Method
cpg	416.91	J/mol×K	697.57	Joback Method
cpg	406.83	J/mol×K	667.62	Joback Method
cpg	396.18	J/mol×K	637.67	Joback Method
cpg	384.91	J/mol×K	607.72	Joback Method
cpg	372.99	J/mol×K	577.77	Joback Method
cpl	372.40	J/mol×K	293.10	NIST Webbook
cpl	372.40	J/mol×K	293.10	NIST Webbook
dvisc	0.0009300	Pa×s	353.15	Density, Viscosity, and Refractive Index in the Range (283.15 to 353.15) K and Vapor Pressure of r-Pinene, d-Limonene, (()-Linalool, and Citral Over the Pressure Range 1.0 kPa Atmospheric Pressure

dvisc	0.0055300	Paxs	293.15	Density, Viscosity, and Refractive Index in the Range (283.15 to 353.15) K and Vapor Pressure of r-Pinene, d-Limonene, (()-Linalool, and Citral Over the Pressure Range 1.0 kPa Atmospheric Pressure
dvisc	0.0011370	Paxs	343.15	Density, Viscosity, and Refractive Index in the Range (283.15 to 353.15) K and Vapor Pressure of r-Pinene, d-Limonene, (()-Linalool, and Citral Over the Pressure Range 1.0 kPa Atmospheric Pressure
dvisc	0.0014320	Paxs	333.15	Density, Viscosity, and Refractive Index in the Range (283.15 to 353.15) K and Vapor Pressure of r-Pinene, d-Limonene, (()-Linalool, and Citral Over the Pressure Range 1.0 kPa Atmospheric Pressure
dvisc	0.0018680	Paxs	323.15	Density, Viscosity, and Refractive Index in the Range (283.15 to 353.15) K and Vapor Pressure of r-Pinene, d-Limonene, (()-Linalool, and Citral Over the Pressure Range 1.0 kPa Atmospheric Pressure

dvisc	0.0025410	Paxs	313.15	Density, Viscosity, and Refractive Index in the Range (283.15 to 353.15) K and Vapor Pressure of r-Pinene, d-Limonene, (()-Linalool, and Citral Over the Pressure Range 1.0 kPa Atmospheric Pressure
dvisc	0.0036300	Paxs	303.15	Density, Viscosity, and Refractive Index in the Range (283.15 to 353.15) K and Vapor Pressure of r-Pinene, d-Limonene, (()-Linalool, and Citral Over the Pressure Range 1.0 kPa Atmospheric Pressure
dvisc	0.0044700	Paxs	298.15	Density, Viscosity, and Refractive Index in the Range (283.15 to 353.15) K and Vapor Pressure of r-Pinene, d-Limonene, (()-Linalool, and Citral Over the Pressure Range 1.0 kPa Atmospheric Pressure
dvisc	0.0090700	Paxs	283.15	Density, Viscosity, and Refractive Index in the Range (283.15 to 353.15) K and Vapor Pressure of r-Pinene, d-Limonene, (()-Linalool, and Citral Over the Pressure Range 1.0 kPa Atmospheric Pressure
hvapt	51.40	kJ/mol	398.00	NIST Webbook
hvapt	50.30	kJ/mol	437.00	NIST Webbook

pvap	0.07	kPa	310.78	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.04	kPa	305.99	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.03	kPa	301.20	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.02	kPa	296.39	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.01	kPa	291.61	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	8.00e-03	kPa	286.91	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	6.42e-03	kPa	284.62	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.01	kPa	289.26	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.02	kPa	294.02	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation

pvap	0.02	kPa	298.77	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.05	kPa	308.38	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.08	kPa	313.18	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.07	kPa	310.74	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.04	kPa	305.95	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.03	kPa	301.14	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.02	kPa	296.39	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.62	kPa	342.71	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation

pvap	0.87	kPa	348.12	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	1.14	kPa	352.90	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.99	kPa	350.51	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.75	kPa	345.69	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.53	kPa	340.29	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.39	kPa	335.48	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.29	kPa	330.68	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.21	kPa	325.83	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.15	kPa	321.01	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation

pvap	0.10	kPa	316.23	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
pvap	0.04	kPa	303.59	Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation
rfi	1.46659		283.15	Thermophysical behaviour of the mixture (+-)-3,7-dimethyl-1,6-octadien-3-ol with ethanol
rfi	1.45950		298.15	Liquid liquid equilibria of the mixture linalool + ethanol +water at different temperatures
rfi	1.44473		328.15	Thermophysical properties of {(+)-linalool + propan-1-ol}: A first stage towards the development of a green process
rfi	1.45215		313.15	Thermophysical properties of {(+)-linalool + propan-1-ol}: A first stage towards the development of a green process
rfi	1.45946		298.15	Thermophysical properties of {(+)-linalool + propan-1-ol}: A first stage towards the development of a green process
rfi	1.46660		283.15	Thermophysical properties of {(+)-linalool + propan-1-ol}: A first stage towards the development of a green process

rfi	1.46659		283.15	Thermophysical properties of {(+)-linalool + propan-1-ol}: A first stage towards the development of a green process	
rfi	1.44473		328.15	Thermophysical behaviour of the mixture (+)-3,7-dimethyl-1,6-octadien-3-ol with ethanol	
rfi	1.45215		313.15	Thermophysical behaviour of the mixture (+)-3,7-dimethyl-1,6-octadien-3-ol with ethanol	
rfi	1.45946		298.15	Thermophysical behaviour of the mixture (+)-3,7-dimethyl-1,6-octadien-3-ol with ethanol	
rfi	1.46660		283.15	Thermophysical behaviour of the mixture (+)-3,7-dimethyl-1,6-octadien-3-ol with ethanol	
rfi	1.46272		293.15	Liquid-Liquid Equilibria of (Limonene + Linalool + Ethylene Glycol or Diethylene Glycol or Triethylene Glycol or 1,2-Propylene Glycol) Ternary Systems	
rfi	1.45961		298.15	Deterpenation of Citrus Essential Oil by Liquid-Liquid Extraction with 1-Alkyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)amide Ionic Liquids	
rhoI	856.83	kg/m3	298.15	Improved concentration of citrus essential oil by solvent extraction with acetate ionic liquids	
rhoI	857.00	kg/m3	298.15	ACSExcess Molar Enthalpies of Mixtures of (+)-Linalool with Several Alkanols	

rho1	857.38	kg/m3	298.20	Physical Behavior of the Phases from the Liquid-Liquid Equilibrium of Citrus Essential Oils Systems at 298.2 K
rho1	856.25	kg/m3	298.20	Deterpenation of Citrus Essential Oils Using Glycerol-Based Deep Eutectic Solvents
rho1	857.38	kg/m3	298.20	Fractionation of orange essential oil using liquid-liquid extraction: Equilibrium data for model and real systems at 298.2 K.

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbp	447.20	K	53.33	Isobaric VLE of the mixture {(+)-linalool + ethanol}: A case study for the distillation of absolute and volatile oils
tbp	406.40	K	13.33	Isobaric VLE of the mixture {(+)-linalool + ethanol}: A case study for the distillation of absolute and volatile oils
tbp	416.80	K	20.00	Isobaric VLE of the mixture {(+)-linalool + ethanol}: A case study for the distillation of absolute and volatile oils

tbp	425.20	K	26.66	Isobaric VLE of the mixture {(+)-linalool + ethanol}: A case study for the distillation of absolute and volatile oils
tbp	432.00	K	33.33	Isobaric VLE of the mixture {(+)-linalool + ethanol}: A case study for the distillation of absolute and volatile oils
tbp	437.80	K	40.00	Isobaric VLE of the mixture {(+)-linalool + ethanol}: A case study for the distillation of absolute and volatile oils
tbp	455.00	K	66.66	Isobaric VLE of the mixture {(+)-linalool + ethanol}: A case study for the distillation of absolute and volatile oils
tbp	461.60	K	79.99	Isobaric VLE of the mixture {(+)-linalool + ethanol}: A case study for the distillation of absolute and volatile oils
tbrp	468.70	K	96.00	NIST Webbook

Datasets

Mass density, kg/m3

Pressure, kPa - Liquid	Temperature, K - Liquid	Mass density, kg/m3 - Liquid
101.80	298.15	857.28

Reference

<https://www.doi.org/10.1016/j.jct.2013.11.026>

Temperature, K	Pressure, kPa	Mass density, kg/m3
293.15	100.00	861.07
Reference		https://www.doi.org/10.1016/j.jct.2016.12.011

Temperature, K	Pressure, kPa	Mass density, kg/m3
298.15	100.00	857.3
Reference		https://www.doi.org/10.1021/acs.jced.8b00939

Temperature, K	Pressure, kPa	Mass density, kg/m3
283.15	100.00	869.2
283.15	5000.00	872.3
283.15	10000.00	875.2
283.15	15000.00	878.2
283.15	20000.00	881.0
283.15	100.00	869.5
283.15	5000.00	872.6
283.15	10000.00	875.7
283.15	15000.00	878.7
283.15	20000.00	881.5
283.18	15000.00	878.7
298.15	100.00	856.9
298.15	5000.00	860.1
298.15	10000.00	863.5
298.15	15000.00	866.6
298.15	20000.00	869.6
298.15	100.00	857.3
298.15	5000.00	860.6
298.15	10000.00	863.9
298.15	15000.00	867.0
298.15	20000.00	870.0
313.15	100.00	844.1
313.15	5000.00	847.8
313.15	10000.00	851.3
313.15	15000.00	854.8
313.15	20000.00	858.1
313.15	100.00	844.5
313.15	5000.00	848.2
313.15	10000.00	851.6

313.15	15000.00	855.0
313.15	20000.00	858.4
328.15	100.00	831.3
328.15	5000.00	835.2
328.15	10000.00	839.1
328.15	15000.00	842.7
328.15	20000.00	846.3
328.15	100.00	831.7
328.15	5000.00	835.6
328.15	10000.00	839.5
328.15	15000.00	843.1
328.15	20000.00	846.7
328.18	10000.00	839.5

Reference

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Physical Properties of Model and Real Systems Composed of Essential Oils and Water: Effect of Ethanol on High-Pressure Vapor-Liquid Equilibria for Supercritical Carbon Dioxide + Linalool + Linalool System: Fractionation of Citrus Essential Oil with using liquid-liquid extraction: Equilibrium data for the water + linalool + limonene) ternary system at T = 298.15, 308.15, and 318.15 K. Alcohols and Ketones: Estimated Solubility Method:

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<https://www.doi.org/10.1021/acs.jced.8b00126>

http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Vapor Liquid Equilibria Measurements of Bitter Orange Aroma Compounds in the Binary System of (Limonene + Hydroxyethyl Glucoside) at 101.3 kPa: Nitroethane or Triethylene Glycol or 1,2-Propylene Glycol Ternary Systems. Behavior of the Phases from the Liquid-Liquid Equilibrium of Citrus Essential Oils Systems at 298.15 K. Aqueous Solubility Prediction Method: extraction: New UNIFAC-VISCO Joback Method:

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https://en.wikipedia.org/wiki/Joback_method

Essential oil deterpenation by solvent extraction using Citrus Essential Oil by liquid-liquid extraction with ionic liquid 1-methyl-3-methylimidazolium hexafluorophosphate (IL) or (1-butyl-3-methylimidazolium hexafluorophosphate) or (1-octyl-3-methylimidazolium hexafluorophosphate) or (1-dodecyl-3-methylimidazolium hexafluorophosphate): A case study for the deterpenation of citrus essential oil by solvent extraction with ionic liquid. Equilibria of the mixture linalool + ethanol + water at different temperatures. Measurements of the (Ethanol + Linalool), (Propan-1-ol + Linalool), and (Propan-2-ol + Linalool) Mixtures: Cubic and Statistical Associating Fluid Theory-Based Equation of State Analyses:

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Deterpenation of Citrus Essential Oils Using Glycerol-Based Deep Eutectic Solvents
 Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 5-methyl-2-hepten-2-one Data in the Range (283.15 to 353.15) K and Vapor Pressure of Enthalpies of McGowan's (V) Linalool, with Several Other Physical properties of Linalool, p. 1-10; A first stage towards the development of a green process:

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<https://www.doi.org/10.1021/je8007414>
<https://www.doi.org/10.1021/je200457q>
<https://www.doi.org/10.1016/j.jct.2010.11.007>

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
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
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
rhof:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbp:	Boiling point at given pressure
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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