

1-Butanol, 3-methyl-, acetate

Other names:	1-Butanol, 3-methyl-, 1-acetate 2-Methylbutyl ethanoate 3-METHYLBUTYL ACETATE 3-METHYLBUTYL ESTER ACETIC ACID 3-Methyl butyl ester acetic acid 3-Methyl-1-butanol acetate 3-Methyl-1-butanyl acetate 3-Methyl-1-butyl acetate 3-Methylbutyl ester of acetic acid 3-Methylbutyl ethanoate 3-methyl-1-butyl acetate (isoamyl acetate) 3-methyl-but-1-yl acetate Acetic acid, 3-methylbutyl ester Acetic acid, isoamyl ester Acetic acid, isopentyl ester Amyl acetate ester Amyl acetate, common Banana oil CH ₃ C(O)O(CH ₂) ₂ CH(CH ₃) ₂ ISOAMYL ACETATE Isoamyl ethanoate Isoamylester kyseliny octove Isopentyl acetate Isopentyl alcohol, acetate Isopentyl alcohol, acetate pear oil Isopentyl ester acetic acid Isopentyl ethanoate Jargonelle pear essence NSC 9260 Pear oil i-Amyl acetate «beta»-Methyl butyl acetate Â«betaÂ»-Methyl butyl acetate
Inchi:	InChI=1S/C7H14O2/c1-6(2)4-5-9-7(3)8/h6H,4-5H2,1-3H3
InchiKey:	MLFHJEHSLIIPHL-UHFFFAOYSA-N
Formula:	C ₇ H ₁₄ O ₂
SMILES:	CC(=O)OCCC(C)C
Mol. weight [g/mol]:	130.18
CAS:	123-92-2

Physical Properties

Property code	Value	Unit	Source
dm	1.80	debye	KDB
gf	-228.30	kJ/mol	Joback Method
hf	-437.89	kJ/mol	Joback Method
hfus	13.15	kJ/mol	Joback Method
hvap	46.40 ± 0.20	kJ/mol	NIST Webbook
log10ws	-1.92		Aqueous Solubility Prediction Method
log10ws	-1.92		Estimated Solubility Method
logp	1.596		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=1)		KDB
pc	2760.00 ± 20.00	kPa	NIST Webbook
rinpol	876.00		NIST Webbook
rinpol	865.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	883.00		NIST Webbook
rinpol	878.00		NIST Webbook
rinpol	876.00		NIST Webbook
rinpol	869.00		NIST Webbook
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ripol	1131.00		NIST Webbook
ripol	1124.00		NIST Webbook
ripol	1126.00		NIST Webbook
ripol	1098.00		NIST Webbook
tb	415.70	K	KDB
tb	415.15	K	Isobaric Vapor-Liquid Equilibrium Measurements for Separation of Azeotrope (Methanol + Methyl Acetate)

tb	415.24	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
tc	599.00	K	KDB
tc	586.10 ± 0.60	K	NIST Webbook
tc	599.33 ± 6.00	K	NIST Webbook
tf	194.60	K	KDB
tf	189.53	K	Aqueous Solubility Prediction Method
vc	0.446	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.45	J/mol×K	615.76	Joback Method
cpg	250.17	J/mol×K	465.47	Joback Method
cpg	261.22	J/mol×K	495.53	Joback Method
cpg	271.87	J/mol×K	525.58	Joback Method
cpg	282.12	J/mol×K	555.64	Joback Method
cpg	291.98	J/mol×K	585.70	Joback Method
cpg	238.73	J/mol×K	435.41	Joback Method
dvisc	0.0006380	Paxs	318.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0006010	Paxs	323.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0005670	Paxs	328.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0005360	Paxs	333.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters

dvisc	0.0005070	Paxs	338.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0006780	Paxs	313.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0009400	Paxs	288.15	Densities and Viscosities of Binary Mixtures of Isoamyl Acetate, Ethyl Caproate, Ethyl Benzoate, Isoamyl Butyrate, Ethyl Phenylacetate, and Ethyl Caprylate with Ethanol at T = (288.15, 298.15, 308.15, and 318.15) K
dvisc	0.0008040	Paxs	298.15	Densities and Viscosities of Binary Mixtures of Isoamyl Acetate, Ethyl Caproate, Ethyl Benzoate, Isoamyl Butyrate, Ethyl Phenylacetate, and Ethyl Caprylate with Ethanol at T = (288.15, 298.15, 308.15, and 318.15) K
dvisc	0.0007040	Paxs	308.15	Densities and Viscosities of Binary Mixtures of Isoamyl Acetate, Ethyl Caproate, Ethyl Benzoate, Isoamyl Butyrate, Ethyl Phenylacetate, and Ethyl Caprylate with Ethanol at T = (288.15, 298.15, 308.15, and 318.15) K

dvisc	0.0006270	Paxs	318.15	Densities and Viscosities of Binary Mixtures of Isoamyl Acetate, Ethyl Caproate, Ethyl Benzoate, Isoamyl Butyrate, Ethyl Phenylacetate, and Ethyl Caprylate with Ethanol at T = (288.15, 298.15, 308.15, and 318.15) K
dvisc	0.0007410	Paxs	303.15	Thermophysical Properties of Isoamyl Acetate or Methyl Benzoate + Hydrocarbon Binary Mixtures, at (303.15 and 313.15) K
dvisc	0.0006490	Paxs	313.15	Thermophysical Properties of Isoamyl Acetate or Methyl Benzoate + Hydrocarbon Binary Mixtures, at (303.15 and 313.15) K
dvisc	0.0007240	Paxs	308.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0007730	Paxs	303.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0008270	Paxs	298.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0008880	Paxs	293.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters

dvisc	0.0007470	Paxs	308.15	Densities, Excess Molar Volumes, Viscosities, Speeds of Sound, Excess Isentropic Compressibilities, and Relative Permittivities for Alkyl (Methyl, Ethyl, Butyl, and Isoamyl) Acetates + Glycols at Different Temperatures
dvisc	0.0004810	Paxs	343.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0007810	Paxs	298.15	Densities, Excess Molar Volumes, Viscosities, Speeds of Sound, Excess Isentropic Compressibilities, and Relative Permittivities for Alkyl (Methyl, Ethyl, Butyl, and Isoamyl) Acetates + Glycols at Different Temperatures
hvapt	44.30	kJ/mol	366.00	NIST Webbook
hvapt	46.80 ± 0.20	kJ/mol	291.50	NIST Webbook
hvapt	45.10	kJ/mol	340.50	NIST Webbook
hvapt	46.40	kJ/mol	332.50	NIST Webbook
pvap	50.00	kPa	391.07	Isobaric Vapor Liquid Equilibria for Binary Mixtures of Isoamyl Acetate + Ethyl Acetate at 50 and 100 kPa
pvap	100.00	kPa	413.46	Isobaric Vapor Liquid Equilibria for Binary Mixtures of Isoamyl Acetate + Ethyl Acetate at 50 and 100 kPa

rfi	1.39760	293.20	Experimental and Correlational Study of Phase Equilibria in Aqueous Solutions of Formic and Butyric Acids with Isoamyl Acetate and Methyl Isoamyl Ketone at T = 298.15 K
rfi	1.39893	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	1.39750	298.15	Application of the ERAS model to volumetric properties of binary mixtures of banana oil with primary and secondary alcohols (C1- C4) at different temperatures
rfi	1.39770	298.15	Isobaric Vapor Liquid Equilibrium for Binary and Ternary Systems of Isoamyl Alcohol + Isoamyl Acetate + Dimethyl Sulfoxide at 101.33 kPa
rfi	1.39842	298.15	Vapor-Liquid Equilibrium Data for Binary Mixtures of Dimethyl Carbonate with Methyl Acetate, Ethyl Acetate, n-Propyl Acetate, Isopropyl Acetate, n-Butyl Acetate, and Isoamyl Acetate at 93.13 kPa

rho1	853.30	kg/m3	313.15	Experimental High-Temperature, High-Pressure Density Measurement and Perturbed-Chain Statistical Associating Fluid Theory Modeling of Dimethyl Sulfoxide, Isoamyl Acetate, and Benzyl Alcohol
rho1	876.00	kg/m3	288.00	KDB
rho1	867.36	kg/m3	298.15	Volumetric Properties of 3-Methylbutyl Ethanoate with Ethyl Acrylate, Butyl Acrylate, Methyl Methacrylate, and Styrene at 25 C
rho1	833.30	kg/m3	333.15	Experimental High-Temperature, High-Pressure Density Measurement and Perturbed-Chain Statistical Associating Fluid Theory Modeling of Dimethyl Sulfoxide, Isoamyl Acetate, and Benzyl Alcohol
rho1	866.70	kg/m3	298.20	Experimental study of phase equilibria in aqueous mixtures of phosphoric acid with isoamyl acetate and methyl isoamyl ketone at T = (298.2, 308.2, and 318.2) K
rho1	872.49	kg/m3	293.20	Liquid-liquid equilibrium data for ternary systems of water + acetic acid + acetate esters at 293.2 K and 303.2 K and ~ 95 kPa

rho1	852.64	kg/m3	313.20	Liquid-liquid equilibrium data for ternary systems of water + acetic acid + acetate esters at 293.2 K and 303.2 K and ~ 95 kPa
rho1	872.90	kg/m3	293.15	Experimental High-Temperature, High-Pressure Density Measurement and Perturbed-Chain Statistical Associating Fluid Theory Modeling of Dimethyl Sulfoxide, Isoamyl Acetate, and Benzyl Alcohol
rho1	868.00	kg/m3	298.15	Experimental High-Temperature, High-Pressure Density Measurement and Perturbed-Chain Statistical Associating Fluid Theory Modeling of Dimethyl Sulfoxide, Isoamyl Acetate, and Benzyl Alcohol
rho1	867.91	kg/m3	298.15	Refractive Indices and Surface Tensions of Binary Mixtures of Isoamyl Acetate, Ethyl Caproate, Ethyl Benzoate, Isoamyl Butyrate, Ethyl Phenylacetate, and Ethyl Caprylate with Ethanol at (288.15, 298.15, 308.15, and 318.15) K
srf	0.02	N/m	358.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K

srf	0.02	N/m	348.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.02	N/m	338.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.02	N/m	328.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.02	N/m	318.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.02	N/m	298.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.03	N/m	288.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.02	N/m	308.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbp	431.61	K	160.01	Vapor Liquid Equilibrium for Binary Mixtures of Acetates in the Direct Esterification of Fusel Oil
tbp	365.29	K	20.00	Vapor Liquid Equilibrium for Binary Mixtures of Acetates in the Direct Esterification of Fusel Oil
tbp	376.06	K	29.98	Vapor Liquid Equilibrium for Binary Mixtures of Acetates in the Direct Esterification of Fusel Oil
tbp	384.31	K	40.01	Vapor Liquid Equilibrium for Binary Mixtures of Acetates in the Direct Esterification of Fusel Oil
tbp	391.07	K	49.99	Vapor Liquid Equilibrium for Binary Mixtures of Acetates in the Direct Esterification of Fusel Oil
tbp	396.76	K	60.00	Vapor Liquid Equilibrium for Binary Mixtures of Acetates in the Direct Esterification of Fusel Oil
tbp	401.72	K	70.00	Vapor Liquid Equilibrium for Binary Mixtures of Acetates in the Direct Esterification of Fusel Oil

tbp	406.18	K	80.01	Vapor Liquid Equilibrium for Binary Mixtures of Acetates in the Direct Esterification of Fusel Oil
tbp	410.24	K	90.00	Vapor Liquid Equilibrium for Binary Mixtures of Acetates in the Direct Esterification of Fusel Oil
tbp	413.90	K	100.01	Vapor Liquid Equilibrium for Binary Mixtures of Acetates in the Direct Esterification of Fusel Oil
tbp	417.15	K	110.00	Vapor Liquid Equilibrium for Binary Mixtures of Acetates in the Direct Esterification of Fusel Oil
tbp	420.43	K	119.99	Vapor Liquid Equilibrium for Binary Mixtures of Acetates in the Direct Esterification of Fusel Oil
tbp	423.46	K	130.00	Vapor Liquid Equilibrium for Binary Mixtures of Acetates in the Direct Esterification of Fusel Oil
tbp	426.33	K	139.99	Vapor Liquid Equilibrium for Binary Mixtures of Acetates in the Direct Esterification of Fusel Oil
tbp	429.05	K	149.99	Vapor Liquid Equilibrium for Binary Mixtures of Acetates in the Direct Esterification of Fusel Oil
tbrp	415.20	K	101.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.53486e+01
Coeff. B	-3.83541e+03
Coeff. C	-5.65620e+01
Temperature range (K), min.	311.22
Temperature range (K), max.	438.68

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	7.60348e+01
Coeff. B	-7.92872e+03
Coeff. C	-8.76739e+00
Coeff. D	3.24333e-06
Temperature range (K), min.	194.65
Temperature range (K), max.	599.00

Datasets

Mass density, kg/m³

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m ³ - Liquid
298.15	100.00	867.3

Reference <https://www.doi.org/10.1021/acs.jced.9b00430>

Sources

Volumetric Properties of 3-Methylbutyl Ethanoate with Ethyl Acrylate, Butyl Acrylate, Methyl Methacrylate, and Styrene at 25 C: <https://www.doi.org/10.1007/s10765-005-5571-9>

Experimental High-Temperature, High-Pressure Density Measurement in Copper Vapor-Liquid Equilibrium Measurements for Separation of Binary and Ternary Systems (Diethyl Carbonate, Isoamyl Acetate, Methyl Acetate): Mixture of Acetates in the Direct Esterification of P-isoamyl acetate in supercritical carbon dioxide. <https://www.doi.org/10.1021/acs.jced.9b00396>

Densities, Excess Molar Volumes, Viscosities, Speeds of Sound, Excess Enthalpy and Viscosity Correlation for Several Common Fragrances and Many Other Scented and Unscented Acetates + Esters of Binary Mixtures of Isoamyl Acetate, Ethyl Caprylate, Ethyl Benzoate, Isoamyl Butyrate, Ethyl Phenylacetate, and Ethyl Caprylate with Ethanol at (288.15, 298.15, 308.15, and 318.15) K. <https://www.doi.org/10.1021/acs.jced.8b00807>

Studies on liquid-liquid interactions of some ternary mixtures by density, viscosity, ultrasonic speed and refractive index measurements: Estimated Solubility Method. <https://www.doi.org/10.1021/acs.jced.6b00221>

Experimental and Correlational Study of Phase Equilibria in Aqueous Solutions of Formic and Butyric Acids with Isoamyl Acetate and Methyl Acetate at T = 298.15 K. <https://www.doi.org/10.1016/j.fluid.2013.12.026>

Phase Equilibria and Thermodynamic Properties of Binary and Ternary Systems of Isoamyl Acetate, Ethyl Caprylate, and Ethyl Benzoate. <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

Phase Equilibria and Thermodynamic Properties of Binary and Ternary Systems of Isoamyl Acetate, Ethyl Caprylate, and Ethyl Benzoate. <https://www.doi.org/10.1021/je0340248>

Phase Equilibria and Thermodynamic Properties of Binary and Ternary Systems of Isoamyl Acetate, Ethyl Caprylate, and Ethyl Benzoate. <https://www.doi.org/10.1021/je050001c>

Phase Equilibria and Thermodynamic Properties of Binary and Ternary Systems of Isoamyl Acetate, Ethyl Caprylate, and Ethyl Benzoate. <https://www.doi.org/10.1021/je0601208>

Phase Equilibria and Thermodynamic Properties of Binary and Ternary Systems of Isoamyl Acetate, Ethyl Caprylate, and Ethyl Benzoate. <https://www.thermopedia.com/research/je0601208>

Phase Equilibria and Thermodynamic Properties of Binary and Ternary Systems of Isoamyl Acetate, Ethyl Caprylate, and Ethyl Benzoate. <https://www.doi.org/10.1016/j.tca.2009.07.011>

Phase Equilibria and Thermodynamic Properties of Binary and Ternary Systems of Isoamyl Acetate, Ethyl Caprylate, and Ethyl Benzoate. <http://webbook.nist.gov/cgi/cbook.cgi?ID=C123922&Units=SI>

Phase Equilibria and Thermodynamic Properties of Binary and Ternary Systems of Isoamyl Acetate, Ethyl Caprylate, and Ethyl Benzoate. http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Phase Equilibria and Thermodynamic Properties of Binary and Ternary Systems of Isoamyl Acetate, Ethyl Caprylate, and Ethyl Benzoate. <https://www.doi.org/10.1021/je401095k>

Phase Equilibria and Thermodynamic Properties of Binary and Ternary Systems of Isoamyl Acetate, Ethyl Caprylate, and Ethyl Benzoate. <http://link.springer.com/article/10.1007/BF02311772>

Phase Equilibria and Thermodynamic Properties of Binary and Ternary Systems of Isoamyl Acetate, Ethyl Caprylate, and Ethyl Benzoate. <https://www.doi.org/10.1021/je0497471>

Phase Equilibria and Thermodynamic Properties of Binary and Ternary Systems of Isoamyl Acetate, Ethyl Caprylate, and Ethyl Benzoate. <https://www.doi.org/10.1016/j.fluid.2018.02.003>

Phase Equilibria and Thermodynamic Properties of Binary and Ternary Systems of Isoamyl Acetate, Ethyl Caprylate, and Ethyl Benzoate. <https://www.doi.org/10.1021/acs.jced.6b00733>

Phase Equilibria and Thermodynamic Properties of Binary and Ternary Systems of Isoamyl Acetate, Ethyl Caprylate, and Ethyl Benzoate. <https://www.doi.org/10.1021/je060321b>

Phase Equilibria and Thermodynamic Properties of Binary and Ternary Systems of Isoamyl Acetate, Ethyl Caprylate, and Ethyl Benzoate. <https://www.doi.org/10.1021/je800325d>

Phase Equilibria and Thermodynamic Properties of Binary and Ternary Systems of Isoamyl Acetate, Ethyl Caprylate, and Ethyl Benzoate. <https://www.doi.org/10.1016/j.jct.2010.12.009>

Phase Equilibria and Thermodynamic Properties of Binary and Ternary Systems of Isoamyl Acetate, Ethyl Caprylate, and Ethyl Benzoate. <https://www.doi.org/10.1021/acs.jced.7b00704>

Phase Equilibria and Thermodynamic Properties of Binary and Ternary Systems of Isoamyl Acetate, Ethyl Caprylate, and Ethyl Benzoate. <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Phase Equilibria and Thermodynamic Properties of Binary and Ternary Systems of Isoamyl Acetate, Ethyl Caprylate, and Ethyl Benzoate. <https://www.doi.org/10.1021/acs.jced.8b01053>

Phase Equilibria and Thermodynamic Properties of Binary and Ternary Systems of Isoamyl Acetate, Ethyl Caprylate, and Ethyl Benzoate. <https://www.doi.org/10.1021/acs.jced.9b00430>

Phase Equilibria and Thermodynamic Properties of Binary and Ternary Systems of Isoamyl Acetate, Ethyl Caprylate, and Ethyl Benzoate. <https://www.doi.org/10.1021/je050170x>

Phase Equilibria and Thermodynamic Properties of Binary and Ternary Systems of Isoamyl Acetate, Ethyl Caprylate, and Ethyl Benzoate. <https://www.doi.org/10.1016/j.fluid.2012.09.038>

Phase Equilibria and Thermodynamic Properties of Binary and Ternary Systems of Isoamyl Acetate, Ethyl Caprylate, and Ethyl Benzoate. <https://www.doi.org/10.1021/je900812v>

Phase Equilibria and Thermodynamic Properties of Binary and Ternary Systems of Isoamyl Acetate, Ethyl Caprylate, and Ethyl Benzoate. <https://www.doi.org/10.1021/acs.jced.6b00197>

Phase Equilibria and Thermodynamic Properties of Binary and Ternary Systems of Isoamyl Acetate, Ethyl Caprylate, and Ethyl Benzoate. <https://www.doi.org/10.1021/je050389b>

Phase Equilibria and Thermodynamic Properties of Binary and Ternary Systems of Isoamyl Acetate, Ethyl Caprylate, and Ethyl Benzoate. <https://www.thermopedia.com/research/kdb/mol/mol1094.mol>

Phase Equilibria and Thermodynamic Properties of Binary and Ternary Systems of Isoamyl Acetate, Ethyl Caprylate, and Ethyl Benzoate. <https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

Legend

cpg:	Ideal gas heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions

h vap:	Enthalpy of vaporization at standard conditions
h vapt:	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
nfpa:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
r fi:	Refractive Index
r hol:	Liquid Density
r inpol:	Non-polar retention indices
r ipol:	Polar retention indices
srf:	Surface Tension
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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