

Acetic acid, propyl ester

Other names:	1-Acetoxypropane
	1-Propyl acetate
	Acetate de propyle normal
	Acetic acid n-propyl ester
	CH ₃ COOCH ₂ CH ₂ CH ₃
	NSC 72025
	Octan propylu
	Propyl ester of acetic acid
	Propylester kyseliny octove
	UN 1276
	ethanoic acid, propyl ester
	n-Propanol acetate
	n-Propyl ethanoate
	n-propyl acetate
	propyl acetate
	propyl ethanoate
Inchi:	InChI=1S/C5H10O2/c1-3-4-7-5(2)6/h3-4H2,1-2H3
InchiKey:	YKYONYBAUNKHLG-UHFFFAOYSA-N
Formula:	C ₅ H ₁₀ O ₂
SMILES:	CCCOC(C)=O
Mol. weight [g/mol]:	102.13
CAS:	109-60-4

Physical Properties

Property code	Value	Unit	Source
af	0.3910		Cheméo Relay (1.0)
affp	836.60	kJ/mol	NIST Webbook
basg	805.60	kJ/mol	NIST Webbook
dvisc	0.0005510	Pa×s	Densities and Viscosities of Ternary Mixtures of Cyclohexane + Cyclohexanone + Some Alkyl Acetates at 298.15 K
gf	-242.70	kJ/mol	Joback Method
hf	-475.14	kJ/mol	Cheméo Relay (1.0)
hfus	11.49	kJ/mol	Joback Method
hvap	39.10 ± 0.20	kJ/mol	NIST Webbook
hvap	34.30 ± 0.04	kJ/mol	NIST Webbook

hvap	39.10 ± 0.20	kJ/mol	NIST Webbook
hvap	39.77	kJ/mol	NIST Webbook
hvap	39.80 ± 0.10	kJ/mol	NIST Webbook
hvap	37.70	kJ/mol	NIST Webbook
ie	9.92	eV	NIST Webbook
ie	10.04 ± 0.03	eV	NIST Webbook
log10ws	-0.72		Aqueous Solubility Prediction Method
log10ws	-0.72		Estimated Solubility Method
logp	0.960		Crippen Method
mccvol	88.750	ml/mol	McGowan Method
pc	3335.00 ± 81.06	kPa	NIST Webbook
pc	3365.10 ± 40.00	kPa	NIST Webbook
pc	3530.00 ± 101.32	kPa	NIST Webbook
rhoc	295.67 ± 5.11	kg/m3	NIST Webbook
rhoc	296.39 ± 4.09	kg/m3	NIST Webbook
rhoc	290.05 ± 6.13	kg/m3	NIST Webbook
rinpol	697.00		NIST Webbook
rinpol	649.00		NIST Webbook
rinpol	694.00		NIST Webbook
rinpol	708.00		NIST Webbook
rinpol	698.00		NIST Webbook
rinpol	713.00		NIST Webbook
rinpol	696.00		NIST Webbook
rinpol	707.00		NIST Webbook
rinpol	728.00		NIST Webbook
rinpol	694.00		NIST Webbook
rinpol	695.00		NIST Webbook
rinpol	708.00		NIST Webbook
rinpol	696.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	695.00		NIST Webbook
rinpol	693.00		NIST Webbook
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rinpol	696.00		NIST Webbook
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rinpol	696.00		NIST Webbook
rinpol	665.00		NIST Webbook
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rinpol	707.00	NIST Webbook
rinpol	717.00	NIST Webbook
rinpol	695.00	NIST Webbook
rinpol	710.00	NIST Webbook
rinpol	695.00	NIST Webbook
rinpol	695.00	NIST Webbook
rinpol	696.30	NIST Webbook
rinpol	684.60	NIST Webbook
rinpol	705.64	NIST Webbook
rinpol	698.31	NIST Webbook
rinpol	708.40	NIST Webbook
rinpol	706.70	NIST Webbook
rinpol	705.40	NIST Webbook
rinpol	676.00	NIST Webbook
rinpol	685.00	NIST Webbook
rinpol	676.00	NIST Webbook
rinpol	696.00	NIST Webbook
rinpol	711.00	NIST Webbook
rinpol	685.00	NIST Webbook
rinpol	695.00	NIST Webbook
rinpol	729.00	NIST Webbook
rinpol	696.00	NIST Webbook
rinpol	693.00	NIST Webbook
rinpol	669.00	NIST Webbook
rinpol	695.80	NIST Webbook
rinpol	653.00	NIST Webbook
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rinpol	695.00	NIST Webbook
rinpol	707.00	NIST Webbook
rinpol	646.00	NIST Webbook
rinpol	695.00	NIST Webbook
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rinpol	654.00	NIST Webbook
rinpol	698.00	NIST Webbook
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rinpol	697.00	NIST Webbook
rinpol	706.00	NIST Webbook
rinpol	682.00	NIST Webbook
rinpol	657.00	NIST Webbook
rinpol	660.00	NIST Webbook
rinpol	708.00	NIST Webbook
rinpol	715.00	NIST Webbook
rinpol	720.10	NIST Webbook
rinpol	682.00	NIST Webbook
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rinpol	735.00	NIST Webbook
rinpol	713.00	NIST Webbook
ripol	957.00	NIST Webbook
ripol	945.00	NIST Webbook
ripol	957.00	NIST Webbook
ripol	968.00	NIST Webbook
ripol	969.00	NIST Webbook
ripol	995.00	NIST Webbook
ripol	944.00	NIST Webbook
ripol	943.00	NIST Webbook
ripol	947.00	NIST Webbook
ripol	990.00	NIST Webbook
ripol	984.00	NIST Webbook
ripol	966.00	NIST Webbook
ripol	945.00	NIST Webbook
ripol	992.00	NIST Webbook
ripol	950.00	NIST Webbook
ripol	975.00	NIST Webbook
ripol	986.00	NIST Webbook
ripol	990.00	NIST Webbook
ripol	990.00	NIST Webbook
ripol	990.00	NIST Webbook
ripol	963.00	NIST Webbook
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ripol	977.00	NIST Webbook
ripol	976.00	NIST Webbook
ripol	935.00	NIST Webbook
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ripol	968.60	NIST Webbook
ripol	970.00	NIST Webbook
ripol	979.00	NIST Webbook
ripol	969.00	NIST Webbook
ripol	971.00	NIST Webbook
ripol	967.00	NIST Webbook
ripol	962.00	NIST Webbook
ripol	943.00	NIST Webbook
ripol	992.00	NIST Webbook
ripol	981.00	NIST Webbook
ripol	978.00	NIST Webbook
ripol	994.00	NIST Webbook
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ripol	969.00	NIST Webbook
ripol	992.00	NIST Webbook
ripol	996.00	NIST Webbook
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ripol	983.00	NIST Webbook
ripol	972.00	NIST Webbook
ripol	952.00	NIST Webbook
ripol	952.00	NIST Webbook
ripol	957.00	NIST Webbook
ripol	928.00	NIST Webbook
ripol	976.00	NIST Webbook
ripol	977.00	NIST Webbook
ripol	992.00	NIST Webbook
ripol	935.00	NIST Webbook
ripol	982.00	NIST Webbook
ripol	939.00	NIST Webbook
ripol	960.00	NIST Webbook
ripol	970.00	NIST Webbook
ripol	995.00	NIST Webbook

ripol	969.00		NIST Webbook
ripol	982.00		NIST Webbook
tb	373.90 ± 1.00	K	NIST Webbook
tb	374.83 ± 0.30	K	NIST Webbook
tb	374.62	K	Isobaric vapor-liquid equilibrium of a ternary system of ethyl acetate + propyl acetate + dimethyl sulfoxide and binary systems of ethyl acetate + dimethyl sulfoxide and propyl acetate + dimethyl sulfoxide at 101.3 kPa
tb	374.65	K	Isobaric Vapor-Liquid Equilibrium for the Binary Systems of 1,2-Dichloroethane + sec-Butyl Acetate, n-Propyl Acetate, and tert-Butyl Acetate at 101.3 kPa
tb	374.80	K	NIST Webbook
tb	374.80	K	Heterogeneous azeotropic distillation for the separation of n-propanol + water mixture using n-propyl acetate as entrainer
tb	374.00	K	NIST Webbook
tb	374.70 ± 0.30	K	NIST Webbook
tb	374.28 ± 0.20	K	NIST Webbook
tb	374.75	K	NIST Webbook
tb	374.62 ± 0.50	K	NIST Webbook
tb	374.20 ± 2.00	K	NIST Webbook
tb	373.95 ± 1.00	K	NIST Webbook
tb	374.85 ± 0.50	K	NIST Webbook
tb	375.00 ± 1.50	K	NIST Webbook
tb	374.75 ± 1.00	K	NIST Webbook
tb	374.62 ± 1.00	K	NIST Webbook
tb	375.15 ± 1.00	K	NIST Webbook
tb	374.70	K	NIST Webbook
tb	373.65 ± 1.00	K	NIST Webbook
tb	373.95 ± 0.50	K	NIST Webbook
tb	374.70 ± 1.00	K	NIST Webbook
tb	375.30 ± 1.00	K	NIST Webbook
tb	374.70 ± 0.50	K	NIST Webbook

tb	374.20	K	Experimental studies and thermodynamic analysis of isobaric vapor-liquid-liquid equilibria of 2-propanol + water system using n-propyl acetate and isopropyl acetate as entrainers
tb	374.80 ± 0.50	K	NIST Webbook
tb	374.80 ± 0.50	K	NIST Webbook
tb	375.65 ± 1.00	K	NIST Webbook
tb	375.20 ± 0.70	K	NIST Webbook
tb	371.00 ± 3.00	K	NIST Webbook
tb	375.13 ± 1.00	K	NIST Webbook
tb	375.00 ± 3.00	K	NIST Webbook
tb	374.69 ± 0.08	K	NIST Webbook
tb	374.75 ± 1.00	K	NIST Webbook
tb	374.75 ± 1.00	K	NIST Webbook
tb	370.65 ± 1.00	K	NIST Webbook
tb	374.50 ± 1.00	K	NIST Webbook
tb	373.00 ± 2.00	K	NIST Webbook
tb	372.65 ± 1.00	K	NIST Webbook
tb	374.80 ± 0.40	K	NIST Webbook
tb	374.75 ± 0.50	K	NIST Webbook
tb	374.75 ± 0.50	K	NIST Webbook
tc	549.40 ± 1.00	K	NIST Webbook
tc	549.73 ± 0.05	K	NIST Webbook
tc	549.40 ± 1.00	K	NIST Webbook
tc	537.70 ± 10.00	K	NIST Webbook
tc	549.50 ± 1.00	K	NIST Webbook
tc	549.40	K	NIST Webbook
tf	179.55	K	Aqueous Solubility Prediction Method
tf	178.15	K	NIST Webbook
tf	178.15 ± 0.60	K	NIST Webbook
vc	0.336	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	153.64	J/mol×K	375.00	NIST Webbook
cpg	162.33	J/mol×K	400.00	NIST Webbook
cpg	171.19	J/mol×K	425.00	NIST Webbook
cpg	178.95	J/mol×K	450.00	NIST Webbook

cpl	194.10	J/mol×K	298.00	NIST Webbook
cpl	196.07	J/mol×K	298.15	NIST Webbook
dvisc	0.0004878	Pa×s	303.15	Densities, Viscosities, and Speeds of Sound of Binary Liquid Mixtures of Sulfolane with Ethyl Acetate, n-Propyl Acetate, and n-Butyl Acetate at Temperature of (303.15, 308.15, and 313.15) K
dvisc	0.0004595	Pa×s	308.15	Densities, Viscosities, and Speeds of Sound of Binary Liquid Mixtures of Sulfolane with Ethyl Acetate, n-Propyl Acetate, and n-Butyl Acetate at Temperature of (303.15, 308.15, and 313.15) K
dvisc	0.0004329	Pa×s	313.15	Densities, Viscosities, and Speeds of Sound of Binary Liquid Mixtures of Sulfolane with Ethyl Acetate, n-Propyl Acetate, and n-Butyl Acetate at Temperature of (303.15, 308.15, and 313.15) K
hvapt	35.30 ± 0.10	kJ/mol	343.00	NIST Webbook
hvapt	33.92	kJ/mol	374.70	NIST Webbook
hvapt	38.60 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	38.10	kJ/mol	352.50	NIST Webbook
hvapt	38.20	kJ/mol	343.00	NIST Webbook
hvapt	34.80	kJ/mol	458.00	NIST Webbook
hvapt	37.00	kJ/mol	352.50	NIST Webbook
hvapt	36.90 ± 0.10	kJ/mol	336.00	NIST Webbook
hvapt	36.40 ± 0.10	kJ/mol	344.00	NIST Webbook
hvapt	35.80 ± 0.10	kJ/mol	351.00	NIST Webbook
hvapt	34.80 ± 0.10	kJ/mol	363.00	NIST Webbook
hvapt	36.90	kJ/mol	335.00	NIST Webbook
hvapt	33.90	kJ/mol	375.00	NIST Webbook
hvapt	36.70	kJ/mol	335.00	NIST Webbook

pvap	34.64	kPa	343.15	Isothermal Vapor-Liquid Equilibria and Excess Enthalpies of (Propyl Ethanoate + Heptane), (Propyl Ethanoate + Cyclohexane), and (Propyl Ethanoate + 1-Hexene)
pvap	91.50	kPa	371.07	Phase equilibria on binary systems containing diethyl sulfide
pvap	23.33	kPa	333.15	Isothermal Vapor-Liquid Equilibria and Excess Enthalpies of (Propyl Ethanoate + Heptane), (Propyl Ethanoate + Cyclohexane), and (Propyl Ethanoate + 1-Hexene)
pvap	23.33	kPa	333.15	Isothermal Vapor-Liquid Equilibria and Excess Enthalpies of (Propyl Ethanoate + Heptane), (Propyl Ethanoate + Cyclohexane), and (Propyl Ethanoate + 1-Hexene)
pvap	22.20	kPa	331.70	Phase equilibria on binary systems containing diethyl sulfide
pvap	50.07	kPa	353.15	Isothermal Vapor-Liquid Equilibria and Excess Enthalpies of (Propyl Ethanoate + Heptane), (Propyl Ethanoate + Cyclohexane), and (Propyl Ethanoate + 1-Hexene)

pvap	50.07	kPa	353.15	Isothermal Vapor-Liquid Equilibria and Excess Enthalpies of (Propyl Ethanoate + Heptane), (Propyl Ethanoate + Cyclohexane), and (Propyl Ethanoate + 1-Hexene)
pvap	70.64	kPa	363.15	Isothermal Vapor-Liquid Equilibria and Excess Enthalpies of (Propyl Ethanoate + Heptane), (Propyl Ethanoate + Cyclohexane), and (Propyl Ethanoate + 1-Hexene)
pvap	70.64	kPa	363.15	Isothermal Vapor-Liquid Equilibria and Excess Enthalpies of (Propyl Ethanoate + Heptane), (Propyl Ethanoate + Cyclohexane), and (Propyl Ethanoate + 1-Hexene)
pvap	16.09	kPa	323.15	Vapor-Liquid Equilibria in the Propyl Acetate + Ethanoic Acid Binary System from (323.15 to 353.15) K: Measurement with a Static Method and Modeling with the NRTL, Wilson, UNIQUAC, and COSMO-SAC Approaches

pvap	24.01	kPa	333.15	Vapor-Liquid Equilibria in the Propyl Acetate + Ethanoic Acid Binary System from (323.15 to 353.15) K: Measurement with a Static Method and Modeling with the NRTL, Wilson, UNIQUAC, and COSMO-SAC Approaches
pvap	34.99	kPa	343.15	Vapor-Liquid Equilibria in the Propyl Acetate + Ethanoic Acid Binary System from (323.15 to 353.15) K: Measurement with a Static Method and Modeling with the NRTL, Wilson, UNIQUAC, and COSMO-SAC Approaches
pvap	49.92	kPa	353.15	Vapor-Liquid Equilibria in the Propyl Acetate + Ethanoic Acid Binary System from (323.15 to 353.15) K: Measurement with a Static Method and Modeling with the NRTL, Wilson, UNIQUAC, and COSMO-SAC Approaches
pvap	31.10	kPa	340.16	Phase equilibria on binary systems containing diethyl sulfide
pvap	41.80	kPa	348.06	Phase equilibria on binary systems containing diethyl sulfide
pvap	50.40	kPa	353.27	Phase equilibria on binary systems containing diethyl sulfide

pvap	62.70	kPa	359.55	Phase equilibria on binary systems containing diethyl sulfide
pvap	71.00	kPa	363.29	Phase equilibria on binary systems containing diethyl sulfide
pvap	81.40	kPa	367.42	Phase equilibria on binary systems containing diethyl sulfide
pvap	15.25	kPa	323.15	Isothermal Vapor-Liquid Equilibria and Excess Enthalpies of (Propyl Ethanoate + Heptane), (Propyl Ethanoate + Cyclohexane), and (Propyl Ethanoate + 1-Hexene)
pvap	101.40	kPa	374.29	Phase equilibria on binary systems containing diethyl sulfide
pvap	101.00	kPa	374.80	Heterogeneous azeotropic distillation for the separation of n-propanol + water mixture using n-propyl acetate as entrainer
pvap	15.25	kPa	323.15	Isothermal Vapor-Liquid Equilibria and Excess Enthalpies of (Propyl Ethanoate + Heptane), (Propyl Ethanoate + Cyclohexane), and (Propyl Ethanoate + 1-Hexene)

pvap	9.65	kPa	313.15	Isothermal Vapor-Liquid Equilibria and Excess Enthalpies of (Propyl Ethanoate + Heptane), (Propyl Ethanoate + Cyclohexane), and (Propyl Ethanoate + 1-Hexene)
pvap	9.64	kPa	313.15	Isothermal Vapor-Liquid Equilibria and Excess Enthalpies of (Propyl Ethanoate + Heptane), (Propyl Ethanoate + Cyclohexane), and (Propyl Ethanoate + 1-Hexene)
pvap	5.87	kPa	303.15	Isothermal Vapor-Liquid Equilibria and Excess Enthalpies of (Propyl Ethanoate + Heptane), (Propyl Ethanoate + Cyclohexane), and (Propyl Ethanoate + 1-Hexene)
pvap	101.00	kPa	374.20	Experimental studies and thermodynamic analysis of isobaric vapor-liquid-liquid equilibria of 2-propanol + water system using n-propyl acetate and isopropyl acetate as entrainers

pvap	101.30	kPa	374.62	Isobaric vapor-liquid equilibrium of a ternary system of ethyl acetate + propyl acetate + dimethyl sulfoxide and binary systems of ethyl acetate + dimethyl sulfoxide and propyl acetate + dimethyl sulfoxide at 101.3 kPa
pvap	101.30	kPa	374.65	Isobaric Vapor-Liquid Equilibrium for the Binary Systems of 1,2-Dichloroethane + sec-Butyl Acetate, n-Propyl Acetate, and tert-Butyl Acetate at 101.3 kPa
pvap	9.59	kPa	313.15	Total Vapor Pressure Measurements for 2-Ethoxyethanol with Methyl Acetate, Ethyl Acetate, Propyl Acetate, and Ethyl Propionate at 313.15 K and for 2-Ethoxyethanol with Methyl Formate at 308.15 K
pvap	0.50	kPa	263.15	Isothermal Vapor-Liquid Equilibria and Excess Enthalpies of (Propyl Ethanoate + Heptane), (Propyl Ethanoate + Cyclohexane), and (Propyl Ethanoate + 1-Hexene)

pvap	1.01	kPa	273.15	Isothermal Vapor-Liquid Equilibria and Excess Enthalpies of (Propyl Ethanoate + Heptane), (Propyl Ethanoate + Cyclohexane), and (Propyl Ethanoate + 1-Hexene)
pvap	1.91	kPa	283.15	Isothermal Vapor-Liquid Equilibria and Excess Enthalpies of (Propyl Ethanoate + Heptane), (Propyl Ethanoate + Cyclohexane), and (Propyl Ethanoate + 1-Hexene)
pvap	3.43	kPa	293.15	Isothermal Vapor-Liquid Equilibria and Excess Enthalpies of (Propyl Ethanoate + Heptane), (Propyl Ethanoate + Cyclohexane), and (Propyl Ethanoate + 1-Hexene)
pvap	4.51	kPa	298.15	Isothermal Vapor-Liquid Equilibria and Excess Enthalpies of (Propyl Ethanoate + Heptane), (Propyl Ethanoate + Cyclohexane), and (Propyl Ethanoate + 1-Hexene)
pvap	4.51	kPa	298.15	Isothermal Vapor-Liquid Equilibria and Excess Enthalpies of (Propyl Ethanoate + Heptane), (Propyl Ethanoate + Cyclohexane), and (Propyl Ethanoate + 1-Hexene)

rfi	1.38280	298.20	Vapor liquid equilibria for the ternary mixture of carbon dioxide + 1-propanol + propyl acetate at elevated pressures
rfi	1.37200	318.15	Multiproperty Correlation of Experimental Data of the Binaries Propyl Ethanoate + Alkanes (Pentane to Decane). New Experimental Information for Vapor Liquid Equilibrium and Mixing Properties
rfi	1.38180	298.15	Multiproperty Correlation of Experimental Data of the Binaries Propyl Ethanoate + Alkanes (Pentane to Decane). New Experimental Information for Vapor Liquid Equilibrium and Mixing Properties
rfi	1.37920	303.15	Correlation and Prediction of Excess Quantities and Vapor-Liquid Equilibria of Alkyl Esters + tert-Butyl Alcohol: Experimental Data for Propyl Esters + tert-Butyl Alcohol
rfi	1.38150	298.15	Isobaric Vapor-Liquid Equilibria of Binary Mixtures of Diethyl Carbonate with Methyl Acetate, n-Propyl Acetate, or Amyl Acetate at 100.17 kPa

rfi	1.38406	298.15	Isobaric Vapor-Liquid Equilibrium Data for Binary Systems of Anisole with Methyl Acetate, Ethyl Acetate, n-Propyl Acetate, and Isopropyl Acetate at 93.9 kPa
rfi	1.38181	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
rfi	1.38300	298.20	Experimental and correlated liquid-liquid equilibrium data for water-phosphoric acid-ester
rfi	1.37410	313.15	Density, refraction index and vapor-liquid equilibria of N-methyl-2-hydroxyethylammonium butyrate plus (methyl acetate or ethyl acetate or propyl acetate) at several temperatures
rfi	1.37210	318.15	Thermodynamic properties of (an ester + an alkane). XVI. Experimental HEm and V Em values and a new correlation method for (an alkyl ethanoate + an n-alkane) at 318.15 K
rfi	1.38210	298.15	Isobaric (vapor+liquid) equilibrium for n-propyl acetate with 1-butanol or 2-butanol. Binary mixtures at 0.15 and 0.6 MPa

rfi	1.37170		318.20	Experimental and calculated liquid-liquid equilibrium data for water + furfural + solvents
rfi	1.37920		303.20	Experimental and calculated liquid-liquid equilibrium data for water + furfural + solvents
rfi	1.38660		288.20	Experimental and calculated liquid-liquid equilibrium data for water + furfural + solvents
rhoI	870.81	kg/m3	308.15	Volumetric Properties of Binary Mixtures of N-Ethylformamide with Tetrahydropyran, 2-Pentanone, and Propylacetate from (293.15 to 313.15) K
rhoI	882.21	kg/m3	298.15	Volumetric Properties of Binary Mixtures of N-Ethylformamide with Tetrahydropyran, 2-Pentanone, and Propylacetate from (293.15 to 313.15) K
rhoI	886.00	kg/m3	298.15	Isobaric Vapor-liquid Equilibrium for Three Binary Systems of Ethyl Acetate + Propyl Acetate, Ethyl Acetate + Propylene Carbonate, and Propyl Acetate + Propylene Carbonate at 101.3 kPa

rhoI	889.00	kg/m3	293.20	Ternary and Quaternary Liquid-Liquid Equilibria for Systems of Methyl Butyl Ketone + Water + Hydroquinone + Phenol at 313.2 K and Atmospheric Pressure
rhoI	881.51	kg/m3	298.20	Liquid-liquid equilibrium for methyl butyl ketone + o-, m-, p-cresol + water ternary systems and COSMO-SAC predictions
rhoI	882.08	kg/m3	298.15	Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) VII. HE m and VE m for 20 binary mixtures {xCu 1H2u 1CO2C3H7 + (1-x)a,x-ClCH2(CH2)v 2CH2Cl}, where u = 1 to 4, a = 1 and v = x = 2 to 6. An analysis of behavior using the COSMO-RS methodology
rhoI	865.21	kg/m3	313.15	Liquid-liquid equilibria and COSMO-SAC modeling of organic solvent/ ionic liquid - hydroxyacetone - water mixtures
rhoI	870.90	kg/m3	308.15	Liquid-liquid equilibria and COSMO-SAC modeling of organic solvent/ ionic liquid - hydroxyacetone - water mixtures
rhoI	876.56	kg/m3	303.15	Liquid-liquid equilibria and COSMO-SAC modeling of organic solvent/ ionic liquid - hydroxyacetone - water mixtures

rhoI	882.19	kg/m3	298.15	Liquid-liquid equilibria and COSMO-SAC modeling of organic solvent/ ionic liquid - hydroxyacetone - water mixtures
rhoI	887.80	kg/m3	293.15	Liquid-liquid equilibria and COSMO-SAC modeling of organic solvent/ ionic liquid - hydroxyacetone - water mixtures
rhoI	876.55	kg/m3	303.15	Excess Volumes and Excess Isentropic Compressibilities of Binary Liquid Mixtures of Trichloroethylene with Esters at 303.15 K
rhoI	883.37	kg/m3	298.15	Volumetric and FT-IR Studies of the Binary Liquid Mixtures of Tributylamine and Alkyl Ester (C1-C5)
rhoI	877.42	kg/m3	303.15	Volumetric and FT-IR Studies of the Binary Liquid Mixtures of Tributylamine and Alkyl Ester (C1-C5)
rhoI	871.78	kg/m3	308.15	Volumetric and FT-IR Studies of the Binary Liquid Mixtures of Tributylamine and Alkyl Ester (C1-C5)
rhoI	866.12	kg/m3	313.15	Volumetric and FT-IR Studies of the Binary Liquid Mixtures of Tributylamine and Alkyl Ester (C1-C5)
rhoI	893.20	kg/m3	288.15	Thermal and Volumetric Properties of Four Aqueous Aroma Compounds at Infinite Dilution

rhoI	882.05	kg/m3	298.15	Thermal and Volumetric Properties of Four Aqueous Aroma Compounds at Infinite Dilution	
rhoI	870.87	kg/m3	308.15	Thermal and Volumetric Properties of Four Aqueous Aroma Compounds at Infinite Dilution	
rhoI	859.52	kg/m3	318.15	Thermal and Volumetric Properties of Four Aqueous Aroma Compounds at Infinite Dilution	
rhoI	887.97	kg/m3	293.15	Volumetric Properties of Binary Mixtures of N-Ethylformamide with Tetrahydropyran, 2-Pentanone, and Propylacetate from (293.15 to 313.15) K	
rhoI	882.40	kg/m3	298.15	Experimental Determination of Vapor Liquid Equilibria. Binary Systems of Methyl Acetate, Ethyl Acetate, and Propyl Acetate with 1-Propanol at 0.6 MPa	
rhoI	864.95	kg/m3	313.15	Volumetric Properties of Binary Mixtures of N-Ethylformamide with Tetrahydropyran, 2-Pentanone, and Propylacetate from (293.15 to 313.15) K	
rhoI	888.96	kg/m3	293.15	Volumetric and FT-IR Studies of the Binary Liquid Mixtures of Tributylamine and Alkyl Ester (C1-C5)	

rhoI	876.54	kg/m3	303.15	Volumetric Properties of Binary Mixtures of N-Ethylformamide with Tetrahydropyran, 2-Pentanone, and Propylacetate from (293.15 to 313.15) K
rhoI	882.80	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
srf	0.02	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
srf	0.02	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	0.02	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

tbp	322.62	K	14.90	Study of Vapor-Liquid Equilibria for Acetic Acid + n-Propyl Acetate + Isopropyl Acetate Systems
tbp	325.01	K	16.60	Study of Vapor-Liquid Equilibria for Acetic Acid + n-Propyl Acetate + Isopropyl Acetate Systems
tbp	327.77	K	18.56	Study of Vapor-Liquid Equilibria for Acetic Acid + n-Propyl Acetate + Isopropyl Acetate Systems
tbp	329.58	K	20.00	Study of Vapor-Liquid Equilibria for Acetic Acid + n-Propyl Acetate + Isopropyl Acetate Systems
tbp	334.71	K	24.75	Study of Vapor-Liquid Equilibria for Acetic Acid + n-Propyl Acetate + Isopropyl Acetate Systems
tbp	337.78	K	27.99	Study of Vapor-Liquid Equilibria for Acetic Acid + n-Propyl Acetate + Isopropyl Acetate Systems
tbp	341.96	K	33.06	Study of Vapor-Liquid Equilibria for Acetic Acid + n-Propyl Acetate + Isopropyl Acetate Systems
tbp	345.55	K	37.76	Study of Vapor-Liquid Equilibria for Acetic Acid + n-Propyl Acetate + Isopropyl Acetate Systems
tbp	347.21	K	40.07	Study of Vapor-Liquid Equilibria for Acetic Acid + n-Propyl Acetate + Isopropyl Acetate Systems

tbp	350.05	K	44.38	Study of Vapor-Liquid Equilibria for Acetic Acid + n-Propyl Acetate + Isopropyl Acetate Systems
tbp	352.73	K	48.69	Study of Vapor-Liquid Equilibria for Acetic Acid + n-Propyl Acetate + Isopropyl Acetate Systems
tbp	355.66	K	54.33	Study of Vapor-Liquid Equilibria for Acetic Acid + n-Propyl Acetate + Isopropyl Acetate Systems
tbp	358.60	K	60.03	Study of Vapor-Liquid Equilibria for Acetic Acid + n-Propyl Acetate + Isopropyl Acetate Systems
tbp	361.80	K	66.87	Study of Vapor-Liquid Equilibria for Acetic Acid + n-Propyl Acetate + Isopropyl Acetate Systems
tbp	364.80	K	73.94	Study of Vapor-Liquid Equilibria for Acetic Acid + n-Propyl Acetate + Isopropyl Acetate Systems
tbp	367.13	K	79.95	Study of Vapor-Liquid Equilibria for Acetic Acid + n-Propyl Acetate + Isopropyl Acetate Systems
tbp	369.07	K	85.25	Study of Vapor-Liquid Equilibria for Acetic Acid + n-Propyl Acetate + Isopropyl Acetate Systems

tbp	371.41	K	91.51	Study of Vapor-Liquid Equilibria for Acetic Acid + n-Propyl Acetate + Isopropyl Acetate Systems
tbp	374.66	K	101.26	Study of Vapor-Liquid Equilibria for Acetic Acid + n-Propyl Acetate + Isopropyl Acetate Systems

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.46116e+01
Coeff. B	-3.24092e+03
Coeff. C	-5.03900e+01
Temperature range (K), min.	276.65
Temperature range (K), max.	398.87

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	9.54327e+01
Coeff. B	-7.93197e+03
Coeff. C	-1.19486e+01
Coeff. D	8.27424e-06
Temperature range (K), min.	178.15
Temperature range (K), max.	549.40

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
298.15	100.00	882.0
298.15	1000.00	882.5
298.15	2000.00	883.4
298.15	3000.00	884.3
298.15	3300.00	884.6
298.15	5000.00	886.4
298.15	10000.00	890.7
298.15	15000.00	894.8
298.15	20000.00	898.7
298.15	25000.00	902.5
298.15	30000.00	906.9
298.15	35000.00	911.7
303.15	100.00	876.2
303.15	1000.00	876.8
303.15	2000.00	877.7
303.15	3000.00	878.8
303.15	3300.00	879.0
303.15	5000.00	880.8
303.15	10000.00	885.3
303.15	15000.00	889.5
303.15	20000.00	893.5
303.15	25000.00	897.4
303.15	30000.00	902.0
303.15	35000.00	906.9
308.15	100.00	870.5
308.15	1000.00	871.2
308.15	2000.00	872.2
308.15	3000.00	873.2
308.15	3300.00	873.4
308.15	5000.00	875.3
308.15	10000.00	879.9
308.15	15000.00	884.3
308.15	20000.00	888.4
308.15	25000.00	892.4
308.15	30000.00	897.2
308.15	35000.00	902.3
313.15	100.00	864.9
313.15	1000.00	865.5
313.15	2000.00	866.6

313.15	3000.00	867.6
313.15	3300.00	867.9
313.15	5000.00	869.9
313.15	10000.00	874.7
313.15	15000.00	879.2
313.15	20000.00	883.5
313.15	25000.00	887.6
313.15	30000.00	892.6
313.15	35000.00	897.7
318.15	100.00	859.3
318.15	1000.00	859.8
318.15	2000.00	860.9
318.15	3000.00	862.1
318.15	3300.00	862.4
318.15	5000.00	864.4
318.15	10000.00	869.4
318.15	15000.00	874.1
318.15	20000.00	878.5
318.15	25000.00	882.8
318.15	30000.00	887.9
318.15	35000.00	893.2
323.15	100.00	853.6
323.15	1000.00	854.8
323.15	2000.00	855.8
323.15	3000.00	856.9
323.15	3300.00	857.1
323.15	5000.00	859.0
323.15	10000.00	864.1
323.15	15000.00	869.0
323.15	20000.00	873.5
323.15	25000.00	877.9
323.15	30000.00	883.2
323.15	35000.00	888.8
328.15	100.00	848.0
328.15	1000.00	848.7
328.15	2000.00	849.9
328.15	3000.00	851.0
328.15	3300.00	851.3
328.15	5000.00	853.7
328.15	10000.00	859.0
328.15	15000.00	864.0
328.15	20000.00	868.7
328.15	25000.00	873.3
328.15	30000.00	878.8

328.15	35000.00	884.4
333.15	100.00	842.5
333.15	1000.00	843.6
333.15	2000.00	844.8
333.15	3000.00	845.9
333.15	3300.00	846.2
333.15	5000.00	848.3
333.15	10000.00	853.9
333.15	15000.00	859.0
333.15	20000.00	863.9
333.15	25000.00	868.6
333.15	30000.00	874.3
333.15	35000.00	880.1
338.15	100.00	836.7
338.15	1000.00	838.0
338.15	2000.00	839.2
338.15	3000.00	840.5
338.15	3300.00	840.8
338.15	5000.00	842.8
338.15	10000.00	848.6
338.15	15000.00	853.9
338.15	20000.00	859.0
338.15	25000.00	863.8
338.15	30000.00	869.6
338.15	35000.00	875.5
343.15	100.00	831.2
343.15	1000.00	832.3
343.15	2000.00	833.7
343.15	3000.00	834.9
343.15	3300.00	835.3
343.15	5000.00	837.6
343.15	10000.00	843.6
343.15	15000.00	849.1
343.15	20000.00	854.3
343.15	25000.00	859.2
343.15	30000.00	865.0
343.15	35000.00	871.2
348.15	100.00	825.6
348.15	1000.00	826.8
348.15	2000.00	828.1
348.15	3000.00	829.5
348.15	3300.00	829.9
348.15	5000.00	832.2
348.15	10000.00	838.3

348.15	15000.00	844.1
348.15	20000.00	849.5
348.15	25000.00	854.5
348.15	30000.00	860.6
348.15	35000.00	866.8
353.15	100.00	820.0
353.15	1000.00	821.2
353.15	2000.00	822.6
353.15	3000.00	824.0
353.15	3300.00	824.4
353.15	5000.00	826.9
353.15	10000.00	833.3
353.15	15000.00	838.8
353.15	20000.00	844.8
353.15	25000.00	850.0
353.15	30000.00	856.4
353.15	35000.00	862.7
358.15	100.00	811.6
358.15	1000.00	812.9
358.15	2000.00	814.4
358.15	3000.00	815.8
358.15	3300.00	816.3
358.15	5000.00	818.6
358.15	10000.00	825.3
358.15	15000.00	831.5
358.15	20000.00	837.2
358.15	25000.00	842.8
363.15	100.00	804.8
363.15	1000.00	806.9
363.15	2000.00	808.4
363.15	3000.00	810.0
363.15	3300.00	810.4
363.15	5000.00	812.9
363.15	10000.00	819.9
363.15	15000.00	826.2
363.15	20000.00	832.1
363.15	25000.00	837.7
363.15	30000.00	844.4
368.15	1000.00	801.0
368.15	2000.00	802.7
368.15	3000.00	804.3
368.15	3300.00	804.8
368.15	5000.00	807.4
368.15	10000.00	814.6

368.15	15000.00	821.2
368.15	20000.00	827.3
368.15	25000.00	833.1
373.15	1000.00	795.5
373.15	2000.00	797.2
373.15	3000.00	798.9
373.15	3300.00	799.5
373.15	5000.00	802.3
373.15	10000.00	809.8
373.15	15000.00	816.6
373.15	20000.00	822.9
373.15	25000.00	828.9
378.15	1000.00	789.4
378.15	2000.00	791.3
378.15	3000.00	793.0
378.15	3300.00	793.6
378.15	5000.00	796.3
378.15	10000.00	803.3
378.15	15000.00	811.3
378.15	20000.00	817.7
378.15	25000.00	824.0
378.15	30000.00	831.2
383.15	1000.00	783.6
383.15	2000.00	785.5
383.15	3000.00	787.3
383.15	3300.00	788.2
383.15	5000.00	791.2
383.15	10000.00	799.2
383.15	15000.00	806.6
383.15	20000.00	813.2
383.15	25000.00	819.7
388.15	1000.00	777.9
388.15	2000.00	779.8
388.15	3000.00	781.6
388.15	3300.00	782.1
388.15	5000.00	785.4
388.15	10000.00	793.8
388.15	15000.00	801.5
388.15	20000.00	808.5
388.15	25000.00	815.2
388.15	30000.00	823.2
393.15	1000.00	771.8
393.15	2000.00	773.9
393.15	3000.00	775.9

Aqueous Solubility Prediction Method:

Isobaric Vapor-Liquid Equilibrium Data for Binary Systems of Anisole with Methyl Acetate, Ethyl Acetate, n-Propyl Acetate, and Isopropyl Acetate at 93.9 kPa for Binary Systems in Equilibrium for the Binary Systems of

K25 Vapor Pressure Data for n-Butyl Acetate, n-Propyl Acetate, and tert-Butyl Acetate (range 1.0):

Legend

<https://www.doi.org/10.1016/j.fluid.2017.05.012>

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
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
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
rhoc:	Critical density
rhoL:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tbp:	Boiling point at given pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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