

Propanoic acid

Other names:	Acide propionique
	Antischim B
	C2H5COOH
	CARBOXYETHANE
	ETHYLFORMIC ACID
	Ethanecarboxylic acid
	Kyselina propionova
	LUPRISOL
	Luprosil
	Metacetonc acid
	Methylacetic acid
	MonoProp
	PROPIONIC ACID
	Propcorn
	Propionic acid grain preserver
	Propkorn
	Prozoin
	Pseudoacetic acid
	Sentry grain preserver
	Tenox P grain preservative
	UN 1848
	n-Propionic acid
Inchi:	InChI=1S/C3H6O2/c1-2-3(4)5/h2H2,1H3,(H,4,5)
InchiKey:	XBDQKXXYIPTUBI-UHFFFAOYSA-N
Formula:	C3H6O2
SMILES:	CCC(=O)O
Mol. weight [g/mol]:	74.08
CAS:	79-09-4

Physical Properties

Property code	Value	Unit	Source
af	0.5200		KDB
affp	797.20	kJ/mol	NIST Webbook
aigt	869.26	K	KDB
basg	766.20	kJ/mol	NIST Webbook
chl	-1528.00	kJ/mol	NIST Webbook

chl	-1527.30 ± 0.10	kJ/mol	NIST Webbook
dm	1.50	debye	KDB
fil	2.90	% in Air	KDB
flu	14.80	% in Air	KDB
fpc	329.82	K	KDB
fpo	327.59	K	KDB
gf	-369.60	kJ/mol	KDB
gyrad	3.0500		KDB
hf	-455.00 ± 3.20	kJ/mol	NIST Webbook
hf	-455.80 ± 2.00	kJ/mol	NIST Webbook
hf	-455.40	kJ/mol	KDB
hf	-455.80 ± 2.00	kJ/mol	NIST Webbook
hfl	-510.80 ± 0.10	kJ/mol	NIST Webbook
hfl	-510.00 ± 2.50	kJ/mol	NIST Webbook
hfus	9.21	kJ/mol	Joback Method
hvap	54.40	kJ/mol	NIST Webbook
hvap	54.90	kJ/mol	NIST Webbook
hvap	55.00	kJ/mol	NIST Webbook
hvap	55.00 ± 2.00	kJ/mol	NIST Webbook
hvap	55.00 ± 2.00	kJ/mol	NIST Webbook
hvap	30.60 ± 0.02	kJ/mol	NIST Webbook
ie	10.72	eV	NIST Webbook
ie	10.51	eV	NIST Webbook
ie	10.44 ± 0.06	eV	NIST Webbook
ie	10.40	eV	NIST Webbook
ie	10.51	eV	NIST Webbook
ie	10.41	eV	NIST Webbook
ie	10.41	eV	NIST Webbook
ie	10.53 ± 0.00	eV	NIST Webbook
ie	10.54	eV	NIST Webbook
ie	10.44 ± 0.03	eV	NIST Webbook
ie	10.24 ± 0.03	eV	NIST Webbook
log10ws	-0.18		Crippen Method
logp	0.481		Crippen Method
mcvol	60.570	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=2)		KDB
pc	4060.00 ± 405.30	kPa	NIST Webbook
pc	4810.14 ± 90.00	kPa	NIST Webbook
pc	4668.00 ± 50.00	kPa	NIST Webbook
pc	4530.00	kPa	KDB
pc	5360.00 ± 506.63	kPa	NIST Webbook
pc	4530.00 ± 50.00	kPa	NIST Webbook
rhoc	334.09 ± 3.33	kg/m3	NIST Webbook

rhoc	314.83 ± 5.93	kg/m3	NIST Webbook
rinpol	702.00		NIST Webbook
rinpol	680.00		NIST Webbook
rinpol	716.00		NIST Webbook
rinpol	716.00		NIST Webbook
rinpol	710.00		NIST Webbook
rinpol	718.00		NIST Webbook
rinpol	700.00		NIST Webbook
rinpol	681.00		NIST Webbook
rinpol	710.00		NIST Webbook
rinpol	693.00		NIST Webbook
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rinpol	725.00		NIST Webbook
rinpol	712.00		NIST Webbook
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rinpol	668.00		NIST Webbook
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rinpol	721.00		NIST Webbook
rinpol	684.00		NIST Webbook
rinpol	745.00		NIST Webbook
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rinpol	700.00		NIST Webbook
rinpol	695.00		NIST Webbook
rinpol	683.00		NIST Webbook
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rinpol	715.00		NIST Webbook

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ripol	1486.00		NIST Webbook
ripol	1525.00		NIST Webbook
ripol	1525.00		NIST Webbook
ripol	1535.00		NIST Webbook
sl	191.00	J/mol×K	NIST Webbook
tb	413.86 ± 0.50	K	NIST Webbook
tb	413.86 ± 0.60	K	NIST Webbook
tb	414.30	K	KDB

tb	414.35	K	Determination and correlation of liquid liquid equilibria for the (water + carboxylic acid + dimethyl maleate) ternary systems at T = 298.2K
tb	413.58	K	Multiphase equilibria for mixtures containing water, isopropanol, propionic acid, and isopropyl propionate
tb	414.25	K	Quaternary phase equilibrium of water-carboxylic acid mixture (formic-propionic acid or acetic-propionic acid)-solvent liquid systems at 298.15 K
tb	414.20	K	Ternary liquid-liquid phase equilibria of (water-carboxylic acid-1-undecanol) systems at 298.15 K
tb	414.01	K	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate and propionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa
tb	414.10	K	(Liquid + liquid) equilibria of (water + propionic acid + dimethyl phthalate) at several temperatures
tb	414.10	K	(Liquid + liquid) equilibria of (water + propionic acid + diethyl phthalate) at several temperatures
tb	414.10	K	(Liquid + liquid) equilibria of (water + propionic acid + cyclohexanone) at several temperatures
tb	414.50	K	(Liquid + liquid) equilibria of (water + propionic acid + alcohol) ternary systems
tb	414.30	K	(Liquid + liquid) equilibria of (water + propionic acid + dipropyl ether or diisopropyl ether) at T = 298.2 K
tb	414.50	K	(Liquid + liquid) equilibria of (water + propionic acid + diethyl succinate or diethyl glutarate or diethyl adipate) ternary systems
tb	414.10	K	(Liquid + liquid) equilibria of (water + propionic acid + 2-ethyl-1-hexanol): Experimental data and correlation

tb	414.32	K	Isobaric vapour-liquid equilibrium for binary systems of ethyl iodide with ethanol, propionic acid and ethyl propionate at 101.3 kPa
tb	414.35	K	Solubility and critical surface in the system propionic acid-ethanol-ethyl propionate-water at 293.15, 303.15 and 313.15 K
tb	414.05	K	Measurements of Quaternary Liquid-Liquid Equilibrium for Water + Acetic Acid + Propionic Acid + Solvent (Butyronitrile, Benzyl Acetate, or Methyl Isobutyl Ketone) at 298.15 K
tb	414.01 ± 0.50	K	NIST Webbook
tb	414.20	K	NIST Webbook
tb	413.85 ± 0.60	K	NIST Webbook
tb	414.50 ± 0.15	K	NIST Webbook
tb	414.50 ± 0.15	K	NIST Webbook
tb	414.15 ± 0.50	K	NIST Webbook
tb	414.00 ± 0.20	K	NIST Webbook
tb	414.10 ± 0.30	K	NIST Webbook
tb	413.90 ± 0.30	K	NIST Webbook
tb	414.20 ± 1.50	K	NIST Webbook
tb	414.00 ± 2.00	K	NIST Webbook
tb	413.95	K	NIST Webbook
tb	414.05 ± 0.50	K	NIST Webbook
tb	414.20 ± 0.20	K	NIST Webbook
tb	413.70 ± 0.40	K	NIST Webbook
tb	413.85 ± 0.40	K	NIST Webbook
tb	414.05 ± 0.20	K	NIST Webbook
tb	414.40 ± 0.30	K	NIST Webbook
tb	412.65 ± 1.00	K	NIST Webbook
tb	414.67 ± 0.40	K	NIST Webbook
tb	414.45 ± 0.50	K	NIST Webbook
tb	412.90 ± 0.60	K	NIST Webbook
tb	414.25 ± 0.50	K	NIST Webbook
tb	414.25 ± 0.60	K	NIST Webbook
tb	414.15 ± 0.50	K	NIST Webbook
tb	413.60 ± 0.40	K	NIST Webbook
tb	414.15 ± 1.50	K	NIST Webbook
tb	413.95 ± 0.30	K	NIST Webbook
tb	414.45 ± 0.50	K	NIST Webbook

tb	410.65 ± 2.00	K	NIST Webbook
tb	413.85 ± 0.30	K	NIST Webbook
tb	414.15 ± 1.00	K	NIST Webbook
tb	414.50 ± 0.50	K	NIST Webbook
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tb	412.65 ± 2.00	K	NIST Webbook
tb	414.45 ± 0.30	K	NIST Webbook
tb	414.60 ± 0.60	K	NIST Webbook
tb	413.85 ± 0.30	K	NIST Webbook
tb	414.65 ± 0.30	K	NIST Webbook
tb	404.15 ± 5.00	K	NIST Webbook
tb	414.15 ± 2.00	K	NIST Webbook
tb	414.40 ± 0.20	K	NIST Webbook
tb	414.95 ± 0.60	K	NIST Webbook
tb	414.50 ± 0.20	K	NIST Webbook
tb	413.25 ± 1.00	K	NIST Webbook
tb	413.10 ± 0.30	K	NIST Webbook
tb	413.85 ± 0.60	K	NIST Webbook
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tb	412.75 ± 1.00	K	NIST Webbook
tb	414.15 ± 1.00	K	NIST Webbook
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tb	412.55 ± 1.00	K	NIST Webbook
tb	415.55 ± 2.00	K	NIST Webbook
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tb	413.85 ± 0.60	K	NIST Webbook
tb	414.05 ± 0.60	K	NIST Webbook
tb	413.95 ± 0.60	K	NIST Webbook
tb	414.00 ± 0.60	K	NIST Webbook
tc	604.00	K	KDB
tc	598.50 ± 1.00	K	NIST Webbook
tc	610.80 ± 6.00	K	NIST Webbook
tc	599.95 ± 1.00	K	NIST Webbook
tc	612.70 ± 6.00	K	NIST Webbook
tc	613.10 ± 6.00	K	NIST Webbook
tc	602.20 ± 2.00	K	NIST Webbook
tc	611.49 ± 2.50	K	NIST Webbook
tc	604.00 ± 0.50	K	NIST Webbook

tf	252.54	K	Solid liquid equilibrium in the ternary system acetic acid propanoic acid formamide
tf	252.32	K	The phase envelopes of alternative solvents (ionic liquid, CO2) and building blocks of biomass origin (lactic acid, propionic acid)
tf	251.95	K	Differential scanning calorimetry determination of phase diagrams and water activities of aqueous carboxylic acid solutions
tf	250.89	K	Determination of the solid liquid phase diagram of the binary system propionic acid / water
tf	252.40	K	KDB
tt	252.65 ± 0.06	K	NIST Webbook
tt	252.65	K	KDB
vc	0.222	m3/kmol	KDB
zc	0.2002520		KDB
zra	0.25		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	121.03	J/mol×K	472.41	Joback Method
cpg	116.00	J/mol×K	443.25	Joback Method
cpg	110.78	J/mol×K	414.09	Joback Method
cpg	139.21	J/mol×K	589.06	Joback Method
cpg	130.50	J/mol×K	530.74	Joback Method
cpg	125.86	J/mol×K	501.57	Joback Method
cpg	134.95	J/mol×K	559.90	Joback Method
cpl	152.80	J/mol×K	298.15	NIST Webbook
cpl	159.40	J/mol×K	289.00	NIST Webbook
cpl	151.00	J/mol×K	298.15	NIST Webbook
cpl	154.60	J/mol×K	333.15	NIST Webbook
cpl	158.60	J/mol×K	298.15	NIST Webbook

dvisc	0.0008476	Pa×s	313.15	Densities and Viscosities of Binary Mixtures of Propanoic Acid with N,N-Dimethylaniline and N,N-Diethylaniline at T = (303.15, 313.15, and 323.15) K
dvisc	0.0007062	Pa×s	323.15	Densities and Viscosities of Binary Mixtures of Propanoic Acid with N,N-Dimethylaniline and N,N-Diethylaniline at T = (303.15, 313.15, and 323.15) K
dvisc	0.0009496	Pa×s	303.15	Densities and Viscosities of Binary Mixtures of Propanoic Acid with N,N-Dimethylaniline and N,N-Diethylaniline at T = (303.15, 313.15, and 323.15) K
hfust	10.66	kJ/mol	252.70	NIST Webbook
hfust	10.66	kJ/mol	252.70	NIST Webbook
hsubt	74.00 ± 1.00	kJ/mol	231.50	NIST Webbook
hsubt	73.00 ± 1.00	kJ/mol	233.00	NIST Webbook
hvapt	46.40	kJ/mol	373.00	NIST Webbook
hvapt	60.60	kJ/mol	462.50	NIST Webbook
hvapt	47.00	kJ/mol	381.00	NIST Webbook
hvapt	56.00	kJ/mol	303.00	NIST Webbook
hvapt	48.30	kJ/mol	382.50	NIST Webbook
pvap	101.30	kPa	414.32	Isobaric vapour-liquid equilibrium for binary systems of ethyl iodide with ethanol, propionic acid and ethyl propionate at 101.3 kPa
pvap	105.30	kPa	415.45	Isobaric (vapour + liquid) equilibria for the (1-pentanol + propionic acid) binary mixture at (53.3 and 91.3) kPa

pvap	14.56	kPa	361.52	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	19.58	kPa	368.37	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	29.65	kPa	378.95	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	39.73	kPa	386.74	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	49.79	kPa	392.93	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid

pvap	59.86	kPa	398.09	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	69.92	kPa	402.65	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	79.99	kPa	406.80	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	90.07	kPa	410.33	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	95.10	kPa	411.97	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid

pvap	101.21	kPa	413.74	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	23.38	kPa	373.10	Vapor-Liquid Equilibria on Four Binary Systems: 2-Phenylpropionaldehyde + Phenol, Propylene Glycol Monomethyl Ether + Nitroethane, Dimethyl Ether + Propylene, and N-Butyric Acid + Propionic Acid
pvap	93.50	kPa	411.65	Isobaric (vapour + liquid) equilibria for the (1-pentanol + propionic acid) binary mixture at (53.3 and 91.3) kPa
pvap	82.50	kPa	407.75	Isobaric (vapour + liquid) equilibria for the (1-pentanol + propionic acid) binary mixture at (53.3 and 91.3) kPa
pvap	71.20	kPa	403.95	Isobaric (vapour + liquid) equilibria for the (1-pentanol + propionic acid) binary mixture at (53.3 and 91.3) kPa
pvap	72.90	kPa	399.05	Isobaric (vapour + liquid) equilibria for the (1-pentanol + propionic acid) binary mixture at (53.3 and 91.3) kPa
pvap	61.80	kPa	393.75	Isobaric (vapour + liquid) equilibria for the (1-pentanol + propionic acid) binary mixture at (53.3 and 91.3) kPa

pvap	51.40	kPa	391.90	Isobaric (vapour + liquid) equilibria for the (1-pentanol + propionic acid) binary mixture at (53.3 and 91.3) kPa
pvap	43.50	kPa	389.10	Isobaric (vapour + liquid) equilibria for the (1-pentanol + propionic acid) binary mixture at (53.3 and 91.3) kPa
pvap	38.30	kPa	385.60	Isobaric (vapour + liquid) equilibria for the (1-pentanol + propionic acid) binary mixture at (53.3 and 91.3) kPa
pvap	34.50	kPa	382.45	Isobaric (vapour + liquid) equilibria for the (1-pentanol + propionic acid) binary mixture at (53.3 and 91.3) kPa
pvap	30.80	kPa	379.65	Isobaric (vapour + liquid) equilibria for the (1-pentanol + propionic acid) binary mixture at (53.3 and 91.3) kPa
pvap	101.30	kPa	413.58	Multiphase equilibria for mixtures containing water, isopropanol, propionic acid, and isopropyl propionate
pvap	96.29	kPa	413.15	Vapor-Liquid Equilibria on Four Binary Systems: 2-Phenylpropionaldehyde + Phenol, Propylene Glycol Monomethyl Ether + Nitroethane, Dimethyl Ether + Propylene, and N-Butyric Acid + Propionic Acid

pvap	112.70	kPa	417.65	Isobaric (vapour + liquid) equilibria for the (1-pentanol + propionic acid) binary mixture at (53.3 and 91.3) kPa
rfi	1.38120		293.15	Vapour-liquid equilibrium of propionic acid + caproic acid, isobutyric acid + caproic acid, valeric acid + caproic acid and caproic acid + enanthoic acid binary mixtures
rfi	1.38290		303.15	Liquid liquid equilibria measurements of ternary systems (acetonitrile + a carboxylic acid + dodecane) at 303.15 K
rfi	1.38290		303.15	Phase equilibria measurements of ternary mixtures (sulfolane + a carboxylic acid + pentane) at 303.15 K
rfi	1.38090		293.15	Isothermal vapour-liquid equilibrium data for the binary systems 2-propanone + (2-butanol or propanoic acid)
rfi	1.38080		293.15	(Liquid + liquid) equilibria of (water + propionic acid + dibasic esters) ternary systems
rfi	1.38110		293.00	Quaternary Liquid-Liquid Equilibrium of Water + Acetic Acid + Propionic Acid + Solvent (Amyl Alcohol, Cyclohexyl Acetate, or Toluene) Systems

rfi	1.38484	298.15	Refractive Index, Surface Tension, and Density of Aqueous Mixtures of Carboxylic Acids at 298.15 K
rfi	1.38610	298.15	Isobaric Vapor-Liquid Equilibria for Binary and Ternary Mixtures of Methanol, Ethanoic Acid, and Propanoic Acid
rfi	1.38580	298.15	Isobaric Vapor-Liquid Equilibria for Binary and Ternary Mixtures of Propanal, Propanol, and Propanoic Acid
rfi	1.38350	293.15	Volumetric Properties of Highly Nonideal Binary Mixtures Containing Ethanoic Acid and Propanoic Acid with Butan-2-ol, Methyl-2-propanol, and 2-Methyl-2-butanol at Different Temperatures
rfi	1.38080	293.15	Liquid phase equilibria of (water + propionic acid + oleyl alcohol) ternary system at several temperatures

rfi	1.38200		298.20	Ternary liquid liquid equilibria for mixtures of an ionic liquid + n-hexane + an organic compound involved in the kinetic resolution of rac-1-phenyl ethanol (rac-1-phenyl ethanol, vinyl propionate, rac-1-phenylethyl propionate or propionic acid) at 298.2K and atmospheric pressure
rfi	1.38110		293.15	(Liquid + liquid) equilibria of (water + propionic acid + methyl isoamyl ketone or diisobutyl ketone or ethyl isoamyl keton) at T = 298.2 K
rfi	1.38110		293.15	Liquid liquid equilibria of ternary systems (water + carboxylic acid + cumene) at 298.15K
rfi	1.38100		293.15	Vapour liquid equilibrium of carboxylic acid systems: Propionic acid + valeric acid and isobutyric acid + valeric acid
rhoI	993.90	kg/m3	293.15	Effect of temperature on density, sound velocity, refractive index and their derived properties for the binary systems (heptanoic acid + propanoic or butanoic acids)

rhoI	960.84	kg/m3	323.15	Experimental Densities and Excess Volumes for Binary Mixtures Containing Propionic Acid, Acetone and Water from 283.15 K to 323.15 K at Atmospheric Pressure
rhoI	993.00	kg/m3	293.00	KDB
rhoI	988.04	kg/m3	298.20	(Liquid + liquid) equilibria of the (water + carboxylic acid + dibasic esters mixture (DBE-2)) ternary systems
rhoI	988.10	kg/m3	298.20	Phase equilibria of (water + propionic acid or butyric acid + 2-methoxy- 2-methylpropane) ternary systems at 298.2 K and 323.2 K
rhoI	993.88	kg/m3	293.15	Density, speed of sound, and refractive index measurements for the binary systems (butanoic acid + propanoic acid, or 2-methyl-propanoic acid) at T = (293.15 to 313.15) K
rhoI	988.48	kg/m3	298.15	Density, speed of sound, and refractive index measurements for the binary systems (butanoic acid + propanoic acid, or 2-methyl-propanoic acid) at T = (293.15 to 313.15) K

rhoI	983.07	kg/m3	303.15	Density, speed of sound, and refractive index measurements for the binary systems (butanoic acid + propanoic acid, or 2-methyl-propanoic acid) at T = (293.15 to 313.15) K
rhoI	977.67	kg/m3	308.15	Density, speed of sound, and refractive index measurements for the binary systems (butanoic acid + propanoic acid, or 2-methyl-propanoic acid) at T = (293.15 to 313.15) K
rhoI	972.27	kg/m3	313.15	Density, speed of sound, and refractive index measurements for the binary systems (butanoic acid + propanoic acid, or 2-methyl-propanoic acid) at T = (293.15 to 313.15) K
rhoI	993.72	kg/m3	298.15	Phase Equilibria for Reactive Distillation of Propyl Propanoate. Pure Component Property Data, Vapor-Liquid Equilibria, and Liquid-Liquid Equilibria
rhoI	988.50	kg/m3	298.15	Effect of temperature on density, sound velocity, refractive index and their derived properties for the binary systems (heptanoic acid + propanoic or butanoic acids)

rhoI	983.10	kg/m3	303.15	Effect of temperature on density, sound velocity, refractive index and their derived properties for the binary systems (heptanoic acid + propanoic or butanoic acids)
rhoI	977.70	kg/m3	308.15	Effect of temperature on density, sound velocity, refractive index and their derived properties for the binary systems (heptanoic acid + propanoic or butanoic acids)
rhoI	972.30	kg/m3	313.15	Effect of temperature on density, sound velocity, refractive index and their derived properties for the binary systems (heptanoic acid + propanoic or butanoic acids)
rhoI	987.90	kg/m3	298.15	Speed of sound as a function of temperature and pressure for propane derivatives
rhoI	998.04	kg/m3	298.15	Liquid Phase Equilibria of Aqueous Mixtures of Carboxylic Acids (C1-C4) with Ethylbenzene: Thermodynamic and Mathematical Modeling
rhoI	988.00	kg/m3	293.15	Correlation of Experimental Liquid Liquid Equilibrium Data for Ternary Systems Using NRTL and GMDH-Type Neural Network

rhoI	993.80	kg/m3	293.15	Probe of Interactions of Acetic and Propionic Acids with 2',3'-N-Epoxypropyl-N-methyl-2-oxopyrrolidinium Salicylate Ionic Liquid
rhoI	988.40	kg/m3	298.15	Probe of Interactions of Acetic and Propionic Acids with 2',3'-N-Epoxypropyl-N-methyl-2-oxopyrrolidinium Salicylate Ionic Liquid
rhoI	983.00	kg/m3	303.15	Probe of Interactions of Acetic and Propionic Acids with 2',3'-N-Epoxypropyl-N-methyl-2-oxopyrrolidinium Salicylate Ionic Liquid
rhoI	977.60	kg/m3	308.15	Probe of Interactions of Acetic and Propionic Acids with 2',3'-N-Epoxypropyl-N-methyl-2-oxopyrrolidinium Salicylate Ionic Liquid
rhoI	966.24	kg/m3	318.14	Experimental Densities and Excess Volumes for Binary Mixtures Containing Propionic Acid, Acetone and Water from 283.15 K to 323.15 K at Atmospheric Pressure
rhoI	1004.11	kg/m3	283.15	Experimental Densities and Excess Volumes for Binary Mixtures Containing Propionic Acid, Acetone and Water from 283.15 K to 323.15 K at Atmospheric Pressure

rhoI	998.69	kg/m3	288.15	Experimental Densities and Excess Volumes for Binary Mixtures Containing Propionic Acid, Acetone and Water from 283.15 K to 323.15 K at Atmospheric Pressure
rhoI	993.26	kg/m3	293.15	Experimental Densities and Excess Volumes for Binary Mixtures Containing Propionic Acid, Acetone and Water from 283.15 K to 323.15 K at Atmospheric Pressure
rhoI	987.85	kg/m3	298.15	Experimental Densities and Excess Volumes for Binary Mixtures Containing Propionic Acid, Acetone and Water from 283.15 K to 323.15 K at Atmospheric Pressure
rhoI	982.44	kg/m3	303.14	Experimental Densities and Excess Volumes for Binary Mixtures Containing Propionic Acid, Acetone and Water from 283.15 K to 323.15 K at Atmospheric Pressure
rhoI	977.04	kg/m3	308.15	Experimental Densities and Excess Volumes for Binary Mixtures Containing Propionic Acid, Acetone and Water from 283.15 K to 323.15 K at Atmospheric Pressure

rhoI	971.63	kg/m3	313.14	Experimental Densities and Excess Volumes for Binary Mixtures Containing Propionic Acid, Acetone and Water from 283.15 K to 323.15 K at Atmospheric Pressure	
rhoI	972.20	kg/m3	313.15	Probe of Interactions of Acetic and Propionic Acids with 2',3'-N-Epoxypropyl-N-methyl-2-oxopyrrolidinium Salicylate Ionic Liquid	
srf	0.03	N/m	308.15	Apparent Molar Volume and Surface Tension of Dilute Aqueous Solutions of Carboxylic Acids	
srf	0.03	N/m	293.15	Apparent Molar Volume and Surface Tension of Dilute Aqueous Solutions of Carboxylic Acids	
srf	0.03	N/m	298.15	Apparent Molar Volume and Surface Tension of Dilute Aqueous Solutions of Carboxylic Acids	
srf	0.03	N/m	303.15	Apparent Molar Volume and Surface Tension of Dilute Aqueous Solutions of Carboxylic Acids	

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
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tbp	368.83	K	20.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate and propionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa
tbp	378.94	K	30.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate and propionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa
tbp	386.59	K	40.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate and propionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa
tbp	392.77	K	50.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate and propionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa
tbp	397.99	K	60.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate and propionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa

tbp	402.56	K	70.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate and propionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa
tbp	406.60	K	80.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate and propionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa
tbp	410.26	K	90.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate and propionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa
tbp	416.68	K	110.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate and propionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa
tbp	419.53	K	120.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate and propionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa

tbp	422.18	K	130.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate and propionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa
tbp	424.67	K	140.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate and propionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa
tbp	427.01	K	150.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate and propionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa
tbp	429.23	K	160.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate and propionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa
tbp	431.36	K	170.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate and propionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa

tbp	433.37	K	180.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate and propionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa
tbp	435.31	K	190.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate and propionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa
tbp	437.16	K	200.00	Vapor-liquid equilibrium of isoamyl alcohol + isoamyl propionate and propionic acid + isoamyl propionate systems at 50.00, 101.33 and 150.00 kPa

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.56739e+01
Coeff. B	-3.98399e+03
Coeff. C	-5.36380e+01
Temperature range (K), min.	312.57
Temperature range (K), max.	600.81

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	7.77767e+01
Coeff. B	-8.37511e+03

Solid liquid equilibrium in the ternary system acetic acid propanoic acid Differential scanning calorimetry determination of Solid-Liquid equilibria phase diagrams for binary mixtures of methyl propanoate and methyl isobutyrate and correlation of surface tension with molecular weight for a series of aliphatic esters: ternary mixtures (sulfolane + a hydrocarbon) at 303.15 K: thermophysical properties of isobutyl acetate in liquid equilibria for binary and ternary mixtures of methyl propanoate and methyl isobutyrate with ethyl iodide equilibria of (water + ethanol), propionitrile and ethyl propionate with cyclohexanone at several temperatures equilibria of (water + propionic acid + dipropyl ether or diisopropyl ether) at 298.2 K: measurements for ternary systems (sulfolane + a hydrocarbon) and surface tension of dilute aqueous solutions of carboxylic acids and correlations of the Vapor Liquid Equilibria for Carbon Monoxide + Propionic Acid and Carbon Monoxide + Methyl Formate Systems: Differential scanning calorimetry determination of phase diagrams and thermophysical properties of such nonideal binary mixtures containing ethanol and ethyl acetate with system propionic acid ethanol-ethyl propionate at 298.15, 303.15, and 308.15 K: Vapor Liquid Equilibria and Surface Tension of Aqueous Mixtures of Carboxylic Acids at 298.15 K: the Quaternary System Toluene + Water + Propionitrile equilibria of (water + propionic acid + dimethyl propionate) at several temperatures: on the dilution enthalpies of carboxylic acids in aqueous solution equilibrium in systems (water + organic solvent + salt) at low water concentrations: phase diagrams of water-carboxylic acid-hydrocarbons and alcohols (1982-1998) thermophysical Properties Databank): (Liquid + liquid) equilibria of (water + propionic acid + alcohol) ternary systems: (liquid + liquid) equilibria of (water + propionic acid + 2-ethyl-1-hexanol): Equilibrium and liquid measurements of ternary systems (acetonitrile + a hydrocarbon) at 298.15, 303.15, 308.15, and 328.2 K: Density, speed of sound, and refractive index measurements for the binary systems (liquid) equilibria of (water + propionitrile + ethyl propionate or propionitrile + ethyl propionate) ternary systems: ethyl propionaldehyde + propionitrile and ethyl propionate + propionitrile and their noncovalent interaction: On the solutions of water in ethyl propionate and ethyl propionate in water and their thermophysical properties for the binary systems liquid equilibrium for Water or Methyl Propanoate or Propionic Acid + Solvent Sulfolane, 2-Ethylpropane and Methylcyclopentanone) at 298.15 K: Vapor-Liquid Equilibrium of carboxylic acid systems: Propionic acid + valeric acid and isobutyric acid + valeric acid: mixtures of (water + propionic acid + organic solvent) at T = 303.2 K:

Liquid-liquid equilibria for ternary systems of (water + carboxylic acid + Phasae equilibria of (water + propionic acid) in butyric acid on 2-methoxypropyl propanoate ternary systems at 298.15 and 323.0 K: liquid + n-hexane + an organic compound involved in the kinetic resolution of rac-1-phenyl ethanol (rac-1-phenyl ethanol, vinyl propionate, rac-1-phenylethyl propionate or propionic acid) at 298.2K and atmospheric pressure:

<https://www.doi.org/10.1016/j.fluid.2007.07.065>
<https://www.doi.org/10.1016/j.fluid.2018.12.035>
<https://www.doi.org/10.1021/je0604277>
<https://www.doi.org/10.1016/j.fluid.2018.07.024>
<https://www.doi.org/10.1016/j.fluid.2015.06.029>
<https://www.doi.org/10.1016/j.jct.2015.05.004>
<https://www.doi.org/10.1021/je100912t>
<https://www.doi.org/10.1016/j.jct.2018.12.023>
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<https://www.doi.org/10.1021/je3001969>
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<https://www.doi.org/10.1016/j.jct.2018.12.026>
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<https://www.doi.org/10.1021/je0496488>
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<https://www.doi.org/10.1016/j.fluid.2014.12.013>
<https://www.doi.org/10.1016/j.tca.2012.04.020>
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<https://www.doi.org/10.1021/je050327l>
<https://www.doi.org/10.1016/j.fluid.2017.05.005>
<https://www.doi.org/10.1016/j.jct.2014.06.004>
<https://www.doi.org/10.1021/je050527x>
<https://www.doi.org/10.1021/je800796h>
<https://www.doi.org/10.1016/j.fluid.2005.08.006>
<https://www.doi.org/10.1016/j.jct.2009.08.014>
https://en.wikipedia.org/wiki/Joback_method
<https://www.doi.org/10.1016/j.fluid.2004.10.029>
<https://www.doi.org/10.1016/j.fluid.2015.06.003>
<https://www.doi.org/10.1016/j.fluid.2007.10.011>

Phase Equilibria for Reactive
 Distillation of Propyl Propanoate. Pure
 (liquid-liquid) equilibria of (water +
 propionic acid + methyl isopropyl ketone
 equilibria of (ketone + ethyl isopropyl
 ketone + 1-chloro-2-chlorophenyl)
 propylamine binary propionic acid +
 water solvent mixtures at 23.2 to
 99.9°C liquid-liquid phase equilibria of isopropyl
 alcohol + isopropyl propionate
 and propionic acid + isopropyl propionate
 acid + caproic acid isobutyric acid +
 caproic acid + isobutyric acid + caproic acid
 and caproic acid + enanthic acid
 measurement and Correlation of the
 Solubility of Florfenicol Form A in
 Several Pure and Binary Solvents
 Liquid Phase Equilibria of (water +
 propionic acid + dibasic esters) ternary
 systems equilibria of (water + carboxylic
 acid + diethyl maleate) ternary liquid
 Determination of the solid liquid phase
 diagram of the binary system propionic
 acid + water
 Liquid phase equilibria of (water +
 propionic acid + oleyl alcohol) ternary
 systems at several temperatures
 Solubilities of α -D-glucose in water +
 (acetic acid or propionic acid))
 Solubility of succinic acid, glutaric acid
 and maleic acid in propionic acid +
 acetic acid mixtures
 Solubility of caproic acid + water mixtures
 the ternary LLE systems of
 the methyl isobutyric acid + isopropyl
 methyl ketone) and of (water +
 propionic acid + D-xylose in water +
 propionic acid or propionic acid) mixtures
 at various pressures and temperatures
 Liquid phase equilibria of (water +
 propionic acid + propionic acid) binary
 mixture at (53.3 and 91.3) kPa:

<https://www.doi.org/10.1021/je101302p>
<https://www.doi.org/10.1016/j.fluid.2006.10.004>
<https://www.doi.org/10.1021/je500291x>
<https://www.doi.org/10.1016/j.fluid.2017.12.023>
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<https://www.doi.org/10.1021/acs.jced.5b00632>
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<https://www.doi.org/10.1016/j.fluid.2012.07.014>
<https://www.doi.org/10.1016/j.jct.2010.05.014>

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
dm:	Dipole Moment
dvisc:	Dynamic viscosity
fill:	Lower Flammability Limit
flu:	Upper Flammability Limit
fpc:	Flash Point (Closed Cup Method)
fpo:	Flash Point (Open Cup Method)
gf:	Standard Gibbs free energy of formation
gyrad:	Radius of Gyration
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
hsbt:	Enthalpy of sublimation 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
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhoc:	Critical density
rhof:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tbp:	Boiling point at given pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility
zra:	Rackett Parameter

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