Pentanoic acid

Other names:	1-Butanecarboxylic acid
	1-Pentanoic acid
	Butanecarboxylic acid
	Kyselina valerova
	N-PENTANOIC ACID
	N-VALERIC ACID
	NA 1760
	NSC 406833
	Propylacetic acid
	VALERIANIC ACID
	Valeric acid
	Valeric acid, n-
	Valeric acid, normal
	n-C4H9COOH
Inchi:	InChI=1S/C5H10O2/c1-2-3-4-5(6)7/h2-4H2,1H3,(H,6,7)
InchiKey:	NQPDZGIKBAWPEJ-UHFFFAOYSA-N
Formula:	C5H10O2
SMILES:	CCCCC(=O)O
Mol. weight [g/mol]:	102.13
CAS:	109-52-4

Physical Properties

Property code	Value	Unit	Source
chl	-2833.40 ± 1.30	kJ/mol	NIST Webbook
chl	-2837.80 ± 0.70	kJ/mol	NIST Webbook
chl	-2850.10 ± 5.90	kJ/mol	NIST Webbook
chl	-2836.50 ± 0.67	kJ/mol	NIST Webbook
chs	-2838.80	kJ/mol	NIST Webbook
gf	-357.40	kJ/mol	KDB
hf	-497.80 ± 4.10	kJ/mol	NIST Webbook
hf	-477.30	kJ/mol	NIST Webbook
hf	-500.90 ± 4.20	kJ/mol	NIST Webbook
hf	-497.80 ± 4.10	kJ/mol	NIST Webbook
hf	-484.20 ± 7.10	kJ/mol	NIST Webbook
hf	-490.70	kJ/mol	KDB
hf	-484.20 ± 7.10	kJ/mol	NIST Webbook
hf	-491.00	kJ/mol	NIST Webbook

hf	-496.50 ± 4.10	kJ/mol	NIST Webbook
hfl	-560.24 ± 0.67	kJ/mol	NIST Webbook
hfl	-563.30 ± 1.30	kJ/mol	NIST Webbook
hfl	-558.90 ± 0.70	kJ/mol	NIST Webbook
hfl	-560.20 ± 0.70	kJ/mol	NIST Webbook
hfl	-546.60 ± 5.90	kJ/mol	NIST Webbook
hfus	14.39	kJ/mol	Joback Method
hvap	50.15	kJ/mol	Joback Method
ie	10.53	eV	NIST Webbook
log10ws	-1.01		Crippen Method
logp	1.261		Crippen Method
mcvol	88.750	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
nfpah	%!d(float64=2)		KDB
pc	3600.00 ± 100.00	kPa	NIST Webbook
pc	3630.00 ± 30.00	kPa	NIST Webbook
pc	3580.00	kPa	KDB
pc	3564.40 ± 90.00	kPa	NIST Webbook
pc	3628.00 ± 40.00	kPa	NIST Webbook
rhoc	300.27 ± 6.13	kg/m3	NIST Webbook
rinpol	137.00		NIST Webbook
rinpol	881.00		NIST Webbook
rinpol	904.00		NIST Webbook
rinpol	872.00		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	878.00		NIST Webbook
rinpol	878.00		NIST Webbook
rinpol	911.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	911.00		NIST Webbook
rinpol	911.00		NIST Webbook
rinpol	879.00		NIST Webbook
rinpol	911.00		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	911.00		NIST Webbook
rinpol	884.00		NIST Webbook
rinpol	875.00		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	892.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	904.00		NIST Webbook
rinpol	875.00		NIST Webbook
rinpol	911.00		NIST Webbook
rinpol	931.00		NIST Webbook

rinpol	867.00	NIST Webbook
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rinpol	906.00	NIST Webbook
rinpol	888.00	NIST Webbook
rinpol	906.00	NIST Webbook
rinpol	906.00	NIST Webbook
rinpol	893.00	NIST Webbook
rinpol	920.00	NIST Webbook
rinpol	887.00	NIST Webbook
rinpol	898.00	NIST Webbook
rinpol	897.00	NIST Webbook
rinpol	924.00	NIST Webbook
rinpol	925.00	NIST Webbook
rinpol	894.00	NIST Webbook
rinpol	938.00	NIST Webbook
rinpol	926.00	NIST Webbook
rinpol	933.30	NIST Webbook
rinpol	902.00	NIST Webbook
rinpol	921.00	NIST Webbook
rinpol	908.00	NIST Webbook
rinpol	921.00	NIST Webbook
rinpol	894.00	NIST Webbook
rinpol	933.00	NIST Webbook
rinpol	925.00	NIST Webbook
rinpol	879.00	NIST Webbook
rinpol	883.00	NIST Webbook
rinpol	888.00	NIST Webbook
rinpol	885.00	NIST Webbook
rinpol	900.00	NIST Webbook
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rinpol	879.00	NIST Webbook
rinpol	878.00	NIST Webbook
rinpol	881.00	NIST Webbook
rinpol	900.00	NIST Webbook
rinpol	933.30	NIST Webbook
rinpol	925.00	NIST Webbook
rinpol	911.00	NIST Webbook
rinpol	883.00	NIST Webbook
rinpol	137.00	NIST Webbook
rinpol	897.00	NIST Webbook
rinpol	906.00	NIST Webbook
rinpol	867.00	NIST Webbook
rinpol	880.00	NIST Webbook

rinpol	921.00	NIST Webbook
ripol	1737.00	NIST Webbook
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ripol	1720.00	NIST Webbook
ripol	1753.00	NIST Webbook
ripol	1721.00	NIST Webbook
ripol	1732.00	NIST Webbook
ripol	1747.00	NIST Webbook
ripol	1706.00	NIST Webbook
ripol	1716.00	NIST Webbook
ripol	1751.00	NIST Webbook
ripol	1753.00	NIST Webbook
ripol	1731.00	NIST Webbook
ripol	1712.00	NIST Webbook
ripol	1723.00	NIST Webbook
ripol	1733.00	NIST Webbook
ripol	1689.00	NIST Webbook
ripol	1737.00	NIST Webbook
ripol	1748.00	NIST Webbook
ripol	1721.00	NIST Webbook
ripol	1746.00	NIST Webbook
ripol	1685.00	NIST Webbook
ripol	1725.00	NIST Webbook
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ripol	1780.00	NIST Webbook
ripol	1736.00	NIST Webbook
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ripol	1734.00		NIST Webbook
ripol	1744.00		NIST Webbook
ripol	1733.00		NIST Webbook
ripol	1685.00		NIST Webbook
ripol	1706.00		NIST Webbook
ripol	1745.00		NIST Webbook
ripol	1730.00		NIST Webbook
sg	439.82 ± 0.63	J/mol×K	NIST Webbook

sl	259.83	J/mol×K	NIST Webbook
tb	459.15	K	Ternary liquid-liquid phase equilibria of (water-carboxylic acid-1-undecanol) systems at 298.15 K
tb	459.30	K	KDB
tc	639.90 ± 0.60	K	NIST Webbook
tc	637.20 ± 1.00	K	NIST Webbook
tc	643.00	K	KDB
tc	652.01 ± 2.50	K	NIST Webbook
tc	643.00 ± 2.00	K	NIST Webbook
tc	637.20 ± 1.00	K	NIST Webbook
tc	652.02 ± 6.00	K	NIST Webbook
tf	238.40 ± 0.60	K	NIST Webbook
tf	239.70 ± 0.10	K	NIST Webbook
tf	239.15 ± 2.00	K	NIST Webbook
tf	239.00	K	KDB
tf	238.65 ± 0.40	K	NIST Webbook
tf	238.70 ± 1.50	K	NIST Webbook
tt	239.49 ± 0.06	K	NIST Webbook
vc	0.340	m3/kmol	KDB
zc	0.2276740		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.15	J/mol×K	574.94	Joback Method
cpg	183.75	J/mol×K	459.85	Joback Method
cpg	226.08	J/mol×K	632.49	Joback Method
cpg	219.76	J/mol×K	603.72	Joback Method
cpg	191.56	J/mol×K	488.62	Joback Method
cpg	199.06	J/mol×K	517.40	Joback Method
cpg	206.25	J/mol×K	546.17	Joback Method
cpl	197.00	J/mol×K	298.15	NIST Webbook
cpl	210.33	J/mol×K	298.15	NIST Webbook
dvisc	0.0078379	Pa×s	290.69	Joback Method
dvisc	0.0002424	Pa×s	459.85	Joback Method
dvisc	0.0006794	Pa×s	392.19	Joback Method
dvisc	0.0272118	Pa×s	256.86	Joback Method
dvisc	0.0013161	Pa×s	358.36	Joback Method
dvisc	0.0029265	Pa×s	324.52	Joback Method

dvisc	0.0003895	Pa×s	426.02	Joback Method
hfust	14.16	kJ/mol	239.49	NIST Webbook
hfust	14.16	kJ/mol	239.50	NIST Webbook
hfust	14.16	kJ/mol	239.50	NIST Webbook
hvapt	57.90	kJ/mol	419.00	NIST Webbook
hvapt	58.00	kJ/mol	449.00	NIST Webbook
pvap	74.96	kPa	448.48	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	85.03	kPa	451.92	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	79.99	kPa	450.35	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	69.92	kPa	446.45	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	59.85	kPa	441.89	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid

pvap	49.78	kPa	436.48	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid	
pvap	39.72	kPa	430.08	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid	
pvap	19.59	kPa	410.71	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid	
pvap	14.56	kPa	403.15	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid	
pvap	29.65	kPa	422.19	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid	

pvap	24.63	kPa	417.07	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
rfi	1.40820		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	1.40870		293.15	Vapour liquid equilibrium of carboxylic acid systems: Propionic acid + valeric acid and isobutyric acid + valeric acid
rfi	1.40470		303.15	Phase equilibria measurements of ternary mixtures (sulfolane + a carboxylic acid + pentane) at 303.15 K
rfi	1.40470		303.15	Liquid liquid equilibria measurements of ternary systems (acetonitrile + a carboxylic acid + dodecane) at 303.15 K
rhol	939.00	kg/m3	293.00	KDB
rhol	831.90	kg/m3	408.30	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhol	812.10	kg/m3	428.20	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K

rhol	939.70	kg/m3	293.40	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhol	921.16	kg/m3	313.15	Influence of alkyl group and temperature on thermophysical properties of carboxylic acid and their binary mixtures
rhol	851.00	kg/m3	388.40	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhol	870.60	kg/m3	368.10	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhol	885.40	kg/m3	352.20	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhol	904.10	kg/m3	332.10	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K
rhol	925.73	kg/m3	308.15	Influence of alkyl group and temperature on thermophysical properties of carboxylic acid and their binary mixtures
rhol	934.85	kg/m3	298.15	Influence of alkyl group and temperature on thermophysical properties of carboxylic acid and their binary mixtures

rhol	939.41	kg/m3	293.15	Influence of alkyl group and temperature on thermophysical properties of carboxylic acid and their binary mixtures	
rhol	934.75	kg/m3	298.15	Liquid-liquid equilibria and density data for pseudoternary systems of refined soybean oil + (hexanal, or heptanal, or butyric acid, or valeric acid, or caproic acid, or caprylic acid) + dimethyl sulfoxide at 298.15 K	
rhol	935.04	kg/m3	298.00	Optimization of liquid-liquid equilibria of the type 2 ternary systems (water + valeric acid + aromatic solvent): Modeling through SERLAS	
rhol	930.29	kg/m3	303.15	Influence of alkyl group and temperature on thermophysical properties of carboxylic acid and their binary mixtures	
rhol	922.30	kg/m3	312.10	Density, Viscosity, and Thermal Conductivity of Eight Carboxylic Acids from (290.3 to 473.4) K	
sfust	59.13	J/mol×K	239.49	NIST Webbook	
srf	0.03	N/m	303.15	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	293.15	Apparent Molar Volume and Surface Tension of Dilute Aqueous Solutions of Carboxylic Acids
srf	0.03	N/m	308.15	Apparent Molar Volume and Surface Tension of Dilute Aqueous Solutions of Carboxylic Acids

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55964e+01
Coeff. B	-4.24155e+03
Coeff. C	-7.26340e+01
Temperature range (K), min.	349.70
Temperature range (K), max.	485.04

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.38077e+01
Coeff. B	-9.69682e+03
Coeff. C	-7.85615e+00
Coeff. D	3.91183e-07
Temperature range (K), min.	239.15
Temperature range (K), max.	651.00

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
298.15	100.00	935.1

Reference *https://www.doi.org/10.1021/acs.jced.8b01189*

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Vapour liquid equilibrium of carboxylic acid systems: Propionic acid + valeric acid and isobutyric acid + valeric acid: https://www.doi.org/10.1016/j.fluid.2005.08.006

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Ternary liquid-liquid phase equilibria of (water-carboxylic acid-1-undecanol) systems at 298.15 K: https://www.doi.org/10.1016/j.fluid.2012.06.020

Effect of temperature on the dilution enthalpies of carboxylic acids in aqueous solutions: https://www.doi.org/10.1016/j.tca.2008.10.013

Liquid-liquid equilibrium of ternary systems comprising ethyl valerate(1), water(2),ethanol(3) and valeric acid(4): https://www.doi.org/10.1016/j.jct.2017.03.030

Phase equilibrium measurements and thermodynamic modelling for the systems involving valeric acid, ethanol, ethyl valerate and water: https://www.doi.org/10.1016/j.jct.2017.05.011

Kirkwood-Buff Integrals, Excess Volume, and Preferential Solvation in Pentanoic Acid/(C5-C10) 1-Alkanol Binary Mixtures: https://www.doi.org/10.1021/acs.jced.8b01189

Conductivity of Eight Carboxylic Acids from (293.15 to 473.47) K: https://www.doi.org/10.1021/acs.jced.5b00971

Phase equilibria measurements of ternary mixtures (sulfolane + a carboxylic acid + pentane) at 303.15 K: https://www.doi.org/10.1016/j.fluid.2015.06.029

Understanding ion-ion and ion-solvent interactions in aqueous solutions of NMF based protic ionic liquids through partial molar properties and DFT calculations: https://www.doi.org/10.1016/j.fluid.2017.05.005

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=934

Differential scanning calorimetry determination of Solid-Liquid equilibria phase diagrams for binary monocarboxylic acids solutions: https://www.doi.org/10.1016/j.fluid.2018.12.035

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

(Liquid + liquid) equilibria measurements for ternary systems (sulfolane + a carboxylic acid + water) at T = 303.15 K and at 0.1 MPa: https://www.doi.org/10.1016/j.jct.2015.12.019

Vapour-liquid equilibrium of propionic acid + caproic acid, isobutyric acid + valeric acid, valeric acid + caproic acid and caproic acid + enanthoic acid binary mixtures: https://www.doi.org/10.1016/j.fluid.2014.04.026

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C109524&Units=SI

Influence of alkyl group and temperature on thermophysical properties of carboxylic acid and their binary mixtures: https://www.doi.org/10.1016/j.tca.2014.06.031

KDB Pure (Korean Thermophysical Properties Databank): https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=934

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid: https://www.doi.org/10.1021/je034180e

Apparent Molar Volume and Surface Tension of Dilute Aqueous Solutions of Valeric Acid: https://www.doi.org/10.1021/je1002829

Liquid-liquid equilibria for the system (water + carboxylic acid + chloroform): https://www.doi.org/10.1016/j.fluid.2006.02.017

Thermodynamic modeling: https://www.doi.org/10.1021/je7007389

Liquid Liquid Equilibria for the Ternary Systems Water + n-Pentanoic Acid with n-Heptane or Dichloromethane at 298.2 K: https://www.doi.org/10.1016/j.jct.2017.12.008

Liquid-liquid equilibria for the aqueous mixture of C5 carboxylic acids and heavier than water solvents at T = 298.2 K:

Liquid-liquid equilibria and density data for pseudoternary systems of refined soybean oil + (hexanal, or heptanal, or butyric acid, or valeric acid, or caproic acid, or caprylic acid) + dimethyl carbonate at 298.15 K:	https://www.doi.org/10.1016/j.jct.2018.10.030
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=934
Phase equilibria of (water + carboxylic acid + diethyl maleate) ternary liquid systems at 298.15 K:	https://www.doi.org/10.1016/j.fluid.2011.01.020
Liquid-liquid equilibria for ternary systems of (water + carboxylic acid + 1-octanol) at 293.15 K: modeling phase equilibria using a solvatochromic approach:	https://www.doi.org/10.1016/j.fluid.2004.10.029
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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Legend

chl:	Standard liquid enthalpy of combustion
chs:	Standard solid enthalpy of combustion
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
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion 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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sg:	Molar entropy at standard conditions
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility