Pentanoic acid, ethyl ester

Other names:	ETHYL ESTER VALERIC ACID
	ETHYL N-VALERATE
	ETHYL PENTANOATE
	Ethyl valerate
	Pentyl propanoate
	Valeric acid, ethyl ester
	n-Valeric acid ethyl ester
Inchi:	InChI=1S/C7H14O2/c1-3-5-6-7(8)9-4-2/h3-6H2,1-2H3
InchiKey:	ICMAFTSLXCXHRK-UHFFFAOYSA-N
Formula:	C7H14O2
SMILES:	CCCCC(=O)OCC
Mol. weight [g/mol]:	130.18
CAS:	539-82-2

Physical Properties

Property code	Value	Unit	Source
chl	-4201.60 ± 2.50	kJ/mol	NIST Webbook
chl	-4202.40 ± 2.50	kJ/mol	NIST Webbook
gf	-225.86	kJ/mol	Joback Method
hf	-507.00 ± 3.00	kJ/mol	NIST Webbook
hf	-507.00 ± 2.00	kJ/mol	NIST Webbook
hf	-507.70	kJ/mol	NIST Webbook
hfl	-554.10 ± 0.80	kJ/mol	NIST Webbook
hfl	-553.80 ± 2.50	kJ/mol	NIST Webbook
hfl	-553.10 ± 8.40	kJ/mol	NIST Webbook
hfus	16.67	kJ/mol	Joback Method
hvap	47.01 ± 0.10	kJ/mol	NIST Webbook
hvap	47.10	kJ/mol	NIST Webbook
hvap	47.00 ± 1.00	kJ/mol	NIST Webbook
hvap	46.00 ± 1.00	kJ/mol	NIST Webbook
hvap	46.10	kJ/mol	NIST Webbook
log10ws	-2.25		Estimated Solubility Method
log10ws	-1.75		Aqueous Solubility Prediction Method
logp	1.740		Crippen Method
mcvol	116.930	ml/mol	McGowan Method

pc	2730.40	kPa	Development of a Predictive Equation of State for CO2 + Ethyl Ester Mixtures Based on Critical Points Measurements
rinpol	878.00		NIST Webbook
rinpol	888.00		NIST Webbook
rinpol	887.00		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	887.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	898.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	904.00		NIST Webbook
rinpol	929.00		NIST Webbook
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rinpol	898.00		NIST Webbook
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rinpol	884.00		NIST Webbook

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ripol	1133.00	NIST Webbook
ripol	1148.00	NIST Webbook
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ripol	1147.00	NIST Webbook
ripol	1141.00	NIST Webbook
ripol	1141.00	NIST Webbook
ripol	1124.00	NIST Webbook
ripol	1138.00	NIST Webbook
ripol	1131.00	NIST Webbook
ripol	1132.00	NIST Webbook
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ripol	1122.00	NIST Webbook

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ripol	1113.00		NIST Webbook
ripol	1159.00		NIST Webbook
ripol	1125.00		NIST Webbook
ripol	1120.00		NIST Webbook
ripol	1131.00		NIST Webbook
ripol	1127.00		NIST Webbook
tb	419.20	K	KDB
tb	417.70 ± 1.00	K	NIST Webbook
tb	417.00 ± 5.00	K	NIST Webbook
tb	417.90 ± 2.00	K	NIST Webbook
tb	407.00 ± 2.00	K	NIST Webbook
tb	417.20 ± 0.40	K	NIST Webbook
tb	417.70	K	NIST Webbook
tb	419.30	K	Ternary phase diagrams for aqueous mixtures of butyric acid with several solvents: experimental and correlated data
tb	408.15 ± 1.50	K	NIST Webbook
tb	418.60 ± 0.25	K	NIST Webbook
tc	593.30 ± 1.00	K	NIST Webbook

tc	570.00	K	KDB
tc	570.20 ± 20.00	K	NIST Webbook
tf	181.90	K	KDB
tf	182.05	K	Aqueous Solubility Prediction Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.48	J/mol×K	582.84	Joback Method
cpg	249.76	J/mol×K	465.25	Joback Method
cpg	260.50	J/mol×K	494.65	Joback Method
cpg	270.86	J/mol×K	524.04	Joback Method
cpg	280.85	J/mol×K	553.44	Joback Method
cpg	238.65	J/mol×K	435.85	Joback Method
cpg	299.73	J/mol×K	612.24	Joback Method
dvisc	0.0004549	Pa×s	370.84	Joback Method
dvisc	0.0006434	Pa×s	338.33	Joback Method
dvisc	0.0002656	Pa×s	435.85	Joback Method
dvisc	0.0016480	Pa×s	273.32	Joback Method
dvisc	0.0031909	Pa×s	240.81	Joback Method
dvisc	0.0003401	Pa×s	403.34	Joback Method
dvisc	0.0009795	Pa×s	305.82	Joback Method
hvapt	38.00	kJ/mol	293.00	NIST Webbook
rfi	1.39800		298.15	Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) I: HE and V E for 25 binary mixtures {xCu-1H2u-1CO2C2H5 + (1-x)a,x-ClCH2(CH2)v-2CH2Cl}, where u = 1 to 5, a = 1 and v = x = 2 to 6

rfi	1.39810		298.15	Correlation and prediction of mixing thermodynamic properties of ester-containing systems: Ester + alkane and ester + ester binary systems and the ternary dodecane + ethyl pentanoate + ethyl ethanoate
rhol	877.15	kg/m3	293.20	Modeling extraction equilibria of butyric acid distributed between water and tri-n-butyl amine/diluent or tri-n-butyl phosphate/diluent system: Extension of the LSER approach
rhol	872.36	kg/m3	298.20	Modeling phase equilibria of ternary systems (water + formic acid + ester or alcohol) through UNIFAC-original, SERLAS, NRTL, NRTL-modified, and three-suffix Margules: Parameter estimation using genetic algorithm
tcondl	0.12	W/m×K	363.57	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.12	W/m×K	358.46	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.12	W/m×K	353.49	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase

tcondl	0.12	W/m×K	348.55	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.12	W/m×K	343.55	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.12	W/m×K	338.47	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.13	W/m×K	333.51	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.13	W/m×K	328.62	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.13	W/m×K	323.74	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.13	W/m×K	318.49	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.13	W/m×K	313.74	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.13	W/m×K	308.61	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.13	W/m×K	303.69	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase

tcondl	0.14	W/m×K	298.79	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.14	W/m×K	293.69	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.14	W/m×K	289.42	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.14	W/m×K	288.74	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.14	W/m×K	283.80	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.14	W/m×K	273.50	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.15	W/m×K	263.90	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.15	W/m×K	249.21	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source

tbp	345.40	K	7.10	Vapor-liquid and liquid-liquid equilibrium modeling of systems involving ethanol, water, and ethyl valerate (valeric acid) using the PC-SAFT equation of state	
tbp	350.70	K	8.90	Vapor-liquid and liquid-liquid equilibrium modeling of systems involving ethanol, water, and ethyl valerate (valeric acid) using the PC-SAFT equation of state	
tbp	361.10	K	13.90	Vapor-liquid and liquid-liquid equilibrium modeling of systems involving ethanol, water, and ethyl valerate (valeric acid) using the PC-SAFT equation of state	
tbp	374.90	K	24.10	Vapor-liquid and liquid-liquid equilibrium modeling of systems involving ethanol, water, and ethyl valerate (valeric acid) using the PC-SAFT equation of state	
tbp	388.30	K	39.10	Vapor-liquid and liquid-liquid equilibrium modeling of systems involving ethanol, water, and ethyl valerate (valeric acid) using the PC-SAFT equation of state	

tbp	395.70	K	52.70	Vapor-liquid and liquid-liquid equilibrium modeling of systems involving ethanol, water, and ethyl valerate (valeric acid) using the PC-SAFT equation of state
tbp	403.90	K	69.30	Vapor-liquid and liquid-liquid equilibrium modeling of systems involving ethanol, water, and ethyl valerate (valeric acid) using the PC-SAFT equation of state
tbp	414.90	K	91.70	Vapor-liquid and liquid-liquid equilibrium modeling of systems involving ethanol, water, and ethyl valerate (valeric acid) using the PC-SAFT equation of state

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53691e+01
Coeff. B	-3.84124e+03
Coeff. C	-5.77010e+01
Temperature range (K), min.	312.40
Temperature range (K), max.	439.62

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	4.34447e+02
Coeff. B	-2.34143e+04

Coeff. C	-6.33502e+01
Coeff. D	5.04777e-05
Temperature range (K), min.	328.15
Temperature range (K), max.	430.15

Datasets

Mass density, kg/m3

Pressure, kPa - Liquid	Temperature, K - Liquid	Mass density, kg/m3 - Liquid
100.00	298.15	870.7
100.00	303.15	865.5
100.00	308.15	860.3
100.00	313.15	855.0
100.00	318.15	849.8
100.00	323.15	844.4
100.00	328.15	839.1
100.00	333.15	833.7
100.00	338.15	828.4
100.00	343.15	823.0
100.00	348.15	817.7
100.00	353.15	812.2
100.00	363.15	801.2
100.00	373.15	790.7
100.00	383.15	779.9
100.00	393.15	769.0
1000.00	298.15	871.5
1000.00	303.15	866.4
1000.00	308.15	861.2
1000.00	313.15	855.9
1000.00	318.15	850.6
1000.00	323.15	845.3
1000.00	328.15	840.0
1000.00	333.15	834.7
1000.00	338.15	829.5
1000.00	343.15	824.1
1000.00	348.15	818.7
1000.00	353.15	813.3
1000.00	363.15	802.5

1000.00	373.15	792.0
1000.00	383.15	781.3
1000.00	393.15	770.5
2000.00	298.15	872.4
2000.00	303.15	867.4
2000.00	308.15	862.1
2000.00	313.15	856.9
2000.00	318.15	851.7
2000.00	323.15	846.4
2000.00	328.15	841.1
2000.00	333.15	836.0
2000.00	338.15	830.7
2000.00	343.15	825.3
2000.00	348.15	820.0
2000.00	353.15	814.6
2000.00	363.15	803.9
2000.00	373.15	793.5
2000.00	383.15	783.0
2000.00	393.15	772.3
2780.00	298.15	873.0
2780.00	303.15	868.1
2780.00	308.15	862.9
2780.00	313.15	857.7
2780.00	318.15	852.4
2780.00	323.15	847.2
2780.00	328.15	842.0
2780.00	333.15	836.9
2780.00	338.15	831.5
2780.00	343.15	826.2
2780.00	348.15	821.0
2780.00	353.15	815.6
2780.00	363.15	805.0
2780.00	373.15	794.7
2780.00	383.15	784.2
2780.00	393.15	773.6
3000.00	298.15	873.2
3000.00	303.15	868.3
3000.00	308.15	863.1
3000.00	313.15	857.9
3000.00	318.15	852.7
3000.00	323.15	847.4
3000.00	328.15	842.3
3000.00	333.15	837.1
3000.00	338.15	831.8

3000.00	343.15	826.5
3000.00	348.15	821.3
3000.00	353.15	815.9
3000.00	363.15	805.5
3000.00	373.15	795.0
3000.00	383.15	784.5
3000.00	393.15	774.1
5000.00	298.15	875.1
5000.00	303.15	870.1
5000.00	308.15	865.0
5000.00	313.15	859.9
5000.00	318.15	854.6
5000.00	323.15	849.4
5000.00	328.15	844.4
5000.00	333.15	839.3
5000.00	338.15	834.0
5000.00	343.15	828.8
5000.00	348.15	823.7
5000.00	353.15	818.4
5000.00	363.15	808.1
5000.00	373.15	797.9
5000.00	383.15	787.6
5000.00	393.15	777.4
10000.00	298.15	879.4
10000.00	303.15	874.5
10000.00	308.15	869.5
10000.00	313.15	864.5
10000.00	318.15	859.4
10000.00	323.15	854.3
10000.00	328.15	849.4
10000.00	333.15	844.5
10000.00	338.15	839.4
10000.00	343.15	834.4
10000.00	348.15	829.4
10000.00	353.15	824.3
10000.00	363.15	814.6
10000.00	373.15	804.8
10000.00	383.15	795.0
10000.00	393.15	785.1
15000.00	298.15	883.4
15000.00	303.15	878.7
15000.00	308.15	873.8
15000.00	313.15	868.9
15000.00	318.15	863.9

15000.00	323.15	859.0
15000.00	328.15	854.2
15000.00	333.15	849.5
15000.00	338.15	844.5
15000.00	343.15	839.6
15000.00	348.15	834.8
15000.00	353.15	829.9
15000.00	363.15	820.5
15000.00	373.15	810.9
15000.00	383.15	801.5
15000.00	393.15	791.6
20000.00	298.15	887.3
20000.00	303.15	882.6
20000.00	308.15	877.8
20000.00	313.15	873.0
20000.00	318.15	868.2
20000.00	323.15	863.4
20000.00	328.15	858.7
20000.00	333.15	854.1
20000.00	338.15	849.3
20000.00	343.15	844.5
20000.00	348.15	839.9
20000.00	353.15	835.1
20000.00	363.15	826.0
20000.00	373.15	816.7
20000.00	383.15	807.6
20000.00	393.15	797.7
25000.00	298.15	891.0
25000.00	303.15	886.5
25000.00	308.15	881.8
25000.00	313.15	877.0
25000.00	318.15	872.3
25000.00	323.15	867.6
25000.00	328.15	863.0
25000.00	333.15	858.6
25000.00	338.15	853.9
25000.00	343.15	849.2
25000.00	348.15	844.7
25000.00	353.15	840.0
25000.00	363.15	831.2
25000.00	373.15	822.2
25000.00	383.15	813.4
25000.00	393.15	803.5
30000.00	298.15	894.6

30000.00	303.15	890.2
30000.00	308.15	885.6
30000.00	313.15	880.9
30000.00	318.15	876.3
30000.00	323.15	871.7
30000.00	328.15	867.1
30000.00	333.15	862.9
30000.00	338.15	858.2
30000.00	343.15	853.7
30000.00	348.15	849.3
30000.00	353.15	844.7
30000.00	363.15	836.0
30000.00	373.15	827.3
30000.00	383.15	818.9
30000.00	393.15	809.0
35000.00	298.15	898.1
35000.00	303.15	893.8
35000.00	308.15	889.2
35000.00	313.15	884.6
35000.00	318.15	880.1
35000.00	323.15	875.5
35000.00	328.15	871.1
35000.00	333.15	867.0
35000.00	338.15	862.4
35000.00	343.15	858.0
35000.00	348.15	853.6
35000.00	353.15	849.1
35000.00	363.15	840.8
35000.00	373.15	832.3
35000.00	383.15	824.0
35000.00	393.15	814.0

Reference *https://www.doi.org/10.1021/je800251v*

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Correlation and prediction of mixing thermodynamic properties of ester containing systems. Ester + alkane and ester + ester binary systems and the ternary n-decane + ethyl pelargonate + ethyl enanthate mixtures	https://www.doi.org/10.1016/j.jct.2012.03.011
Ternary phase diagrams for aqueous mixtures of butyric acid with several [illegible] systems and the ternary n-decane + ethyl pelargonate + ethyl enanthate	https://www.doi.org/10.1016/j.fluid.2014.03.008
Development of a Predictive Equation of State for CO2 + Ethyl Ester Mixtures Based on Critical Points	https://www.doi.org/10.1021/je5002494
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Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas 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
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbp:	Boiling point at given pressure
tc:	Critical Temperature
tcondl:	Liquid thermal conductivity

tf:	Normal melting (fusion) point
vc:	Critical Volume