Propanoic acid, ethyl ester

Other names:	C2H5COOC2H5
	ETHYL ESTER PROPIONIC ACID
	Ethyl ester of propanoic acid
	Ethyl n-propionate
	Ethyl propanoate
	Ethyl propionate
	Ethylester kyseliny propionove
	NSC 8848
	Propionate d'ethyle
	Propionic acid, ethyl ester
	Propionic ester
	Propionic ether
	UN 1195
	n-Ethyl propanoate
Inchi:	InChI=1S/C5H10O2/c1-3-5(6)7-4-2/h3-4H2,1-2H3
InchiKey:	FKRCODPIKNYEAC-UHFFFAOYSA-N
Formula:	C5H10O2
SMILES:	CCOC(=O)CC
Mol. weight [g/mol]:	102.13
CAS:	105-37-3

Physical Properties

Property code	Value	Unit	Source
af	0.3910		KDB
chl	-2888.00	kJ/mol	NIST Webbook
chl	-2912.10 ± 2.00	kJ/mol	NIST Webbook
chl	-2894.00 ± 0.65	kJ/mol	NIST Webbook
dm	1.80	debye	KDB
gf	-323.70	kJ/mol	KDB
hf	-466.50 ± 0.40	kJ/mol	NIST Webbook
hf	-470.20	kJ/mol	KDB
hf	-463.60 ± 0.70	kJ/mol	NIST Webbook
hfl	-502.70 ± 0.70	kJ/mol	NIST Webbook
hfl	-505.59 ± 0.50	kJ/mol	NIST Webbook
hfus	11.49	kJ/mol	Joback Method
hvap	35.88	kJ/mol	Joback Method
ie	10.00 ± 0.02	eV	NIST Webbook

log10ws	-0.66		Aqueous Solubility Prediction Method
log10ws	-0.66		Estimated Solubility Method
logp	0.959		Crippen Method
mcvol	88.750	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
pc	3385.60	kPa	Development of a Predictive Equation of State for CO2 + Ethyl Ester Mixtures Based on Critical Points Measurements
pc	3359.70 ± 40.00	kPa	NIST Webbook
pc	3362.00 ± 81.06	kPa	NIST Webbook
pc	3510.00 ± 202.65	kPa	NIST Webbook
pc	3510.00 ± 202.65	kPa	NIST Webbook
pc	3362.00	kPa	KDB
rhoc	285.97 ± 10.01	kg/m3	NIST Webbook
rhoc	285.97 ± 10.01	kg/m3	NIST Webbook
rhoc	296.90 ± 4.09	kg/m3	NIST Webbook
rhoc	296.49 ± 10.01	kg/m3	NIST Webbook
rinpol	705.00		NIST Webbook
rinpol	663.00		NIST Webbook
rinpol	715.00		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	694.20		NIST Webbook
rinpol	684.00		NIST Webbook
rinpol	694.00		NIST Webbook
rinpol	695.00		NIST Webbook
rinpol	694.20		NIST Webbook
rinpol	678.95		NIST Webbook
rinpol	700.00		NIST Webbook
rinpol	678.00		NIST Webbook
rinpol	692.00		NIST Webbook
rinpol	684.00		NIST Webbook
rinpol	688.00		NIST Webbook
rinpol	695.00		NIST Webbook
rinpol	707.00		NIST Webbook
rinpol	685.00		NIST Webbook
rinpol	694.00		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	694.00		NIST Webbook
rinpol	692.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	695.00		NIST Webbook

rinpol	679.00	NIST Webbook
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rinpol	685.00	NIST Webbook
rinpol	706.00	NIST Webbook
rinpol	692.00	NIST Webbook
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rinpol	714.00	NIST Webbook
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rinpol	705.00	NIST Webbook
rinpol	680.00	NIST Webbook
rinpol	681.00	NIST Webbook
rinpol	714.00	NIST Webbook
rinpol	696.00	NIST Webbook
rinpol	681.00	NIST Webbook
rinpol	681.00	NIST Webbook
rinpol	711.00	NIST Webbook
rinpol	691.00	NIST Webbook
rinpol	712.00	NIST Webbook
rinpol	700.00	NIST Webbook
rinpol	708.00	NIST Webbook
rinpol	726.00	NIST Webbook
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rinpol	702.00	NIST Webbook
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rinpol	714.00	NIST Webbook
rinpol	690.00	NIST Webbook
rinpol	729.00	NIST Webbook

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rinpol	695.00	NIST Webbook
rinpol	703.00	NIST Webbook
rinpol	703.00	NIST Webbook
rinpol	705.00	NIST Webbook
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ripol	953.00	NIST Webbook
ripol	955.00	NIST Webbook
ripol	976.00	NIST Webbook
ripol	957.00	NIST Webbook
ripol	939.00	NIST Webbook
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ripol	974.00		NIST Webbook
ripol	964.00		NIST Webbook
ripol	961.00		NIST Webbook
ripol	957.00		NIST Webbook
ripol	959.00		NIST Webbook
ripol	960.00		NIST Webbook
ripol	944.00		NIST Webbook
tb	372.20	K	KDB
tb	372.25	K	Solubility and critical surface in the system propionic acid-ethanol-ethyl propionate-water at 293.15, 303.15 and 313.15 K
tb	372.25	K	Isobaric vapour-liquid equilibrium for binary systems of ethyl iodide with ethanol, propionic acid and ethyl propionate at 101.3 kPa
tb	372.20	K	(Liquid + liquid) equilibria of (water + butyric acid + esters) ternary systems
tb	371.91	K	Isobaric Vapor-Liquid Equilibria and Excess Quantities for Binary Mixtures of an Ethyl Ester + tert-Butanol and a New Approach to VLE Data Processing
tc	546.10 ± 1.00	K	NIST Webbook
tc	545.60 ± 1.00	K	NIST Webbook
tc	552.70 ± 5.00	K	NIST Webbook
tc	545.60 ± 2.00	K	NIST Webbook
tc	553.80 ± 5.00	K	NIST Webbook
tc	546.00	K	NIST Webbook
tc	546.00	K	KDB

tc	546.00 ± 1.00	K	NIST Webbook
tf	199.25 ± 0.40	K	NIST Webbook
tf	200.24 ± 0.20	K	NIST Webbook
tf	199.71	K	Efficient determination of crystallisation and melting points at low cooling and heating rates with novel computer controlled equipment
tf	199.20	K	KDB
tf	199.85	K	Aqueous Solubility Prediction Method
vc	0.345	m3/kmol	KDB
zc	0.2554980		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	171.91	J/mol×K	419.85	Joback Method
cpg	210.46	J/mol×K	568.66	Joback Method
cpg	203.26	J/mol×K	538.90	Joback Method
cpg	195.80	J/mol×K	509.14	Joback Method
cpg	188.08	J/mol×K	479.38	Joback Method
cpg	180.12	J/mol×K	449.61	Joback Method
cpg	163.46	J/mol×K	390.09	Joback Method
cpl	200.90	J/mol×K	298.15	NIST Webbook
cpl	199.58	J/mol×K	298.33	NIST Webbook
dvisc	0.0004920	Pa×s	298.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0003290	Pa×s	338.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0003440	Pa×s	333.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters

dvisc	0.0003600	Pa×s	328.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0003780	Pa×s	323.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0005230	Pa×s	293.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0004180	Pa×s	313.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0004410	Pa×s	308.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0004640	Pa×s	303.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0003150	Pa×s	343.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0003980	Pa×s	318.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
hvapt	33.88	kJ/mol	372.20	NIST Webbook
hvapt	36.70	kJ/mol	367.50	NIST Webbook
hvapt	38.20 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	36.60 ± 0.10	kJ/mol	336.00	NIST Webbook
hvapt	36.00 ± 0.10	kJ/mol	344.00	NIST Webbook
hvapt	35.50 ± 0.10	kJ/mol	351.00	NIST Webbook
hvapt	34.50 ± 0.10	kJ/mol	363.00	NIST Webbook
hvapt	38.20	kJ/mol	339.00	NIST Webbook
hvapt	34.40	kJ/mol	455.00	NIST Webbook

pvap	10.60	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	101.30	kPa	372.25	Isobaric vapour-liquid equilibrium for binary systems of ethyl iodide with ethanol, propionic acid and ethyl propionate at 101.3 kPa	
rfi	1.38110		298.15	Improvements in the Experimentation and the Representation of Thermodynamic Properties (iso-p VLE and yE) of Alkyl Propanoate + Alkane Binaries	
rfi	1.38150		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	1.37110		318.15	Thermodynamic properties of (an ester + and alkane). XVII. Experimental He and Ve values for (an alkyl propanoate + an alkane) at 318.15K	
rhol	895.00	kg/m3	289.00	KDB	

tcondl	0.12	W/m×K	356.28	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.13	W/m×K	321.47	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.13	W/m×K	316.45	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.13	W/m×K	311.34	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.14	W/m×K	306.51	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.14	W/m×K	301.40	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.14	W/m×K	296.36	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.13	W/m×K	326.44	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.14	W/m×K	293.54	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.14	W/m×K	288.56	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase

tcondl	0.14	W/m×K	283.51	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.15	W/m×K	278.51	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.15	W/m×K	270.94	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.15	W/m×K	268.41	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.13	W/m×K	331.53	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.13	W/m×K	336.40	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.12	W/m×K	341.36	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.12	W/m×K	346.42	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.12	W/m×K	351.35	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase
tcondl	0.15	W/m×K	263.55	Measurement of the thermal conductivity of five aliphatic esters in the liquid phase

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45526e+01
Coeff. B	-3.16736e+03
Coeff. C	-5.33670e+01
Temperature range (K), min.	275.40
Temperature range (K), max.	396.11

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.01207e+02
Coeff. B	-8.10148e+03
Coeff. C	-1.28594e+01
Coeff. D	9.33835e-06
Temperature range (K), min.	199.25
Temperature range (K), max.	546.00

Datasets

Mass density, kg/m3

Pressure, kPa - Liquid	Temperature, K - Liquid	Mass density, kg/m3 - Liquid
100.00	298.15	884.3
100.00	303.15	878.5
100.00	308.15	872.7
100.00	313.15	866.8
100.00	318.15	860.9
100.00	323.15	854.9
100.00	328.15	849.2
100.00	333.15	843.1
100.00	338.15	836.9

100.00	343.15	831.1
100.00	348.15	824.9
100.00	353.15	818.7
100.00	363.15	803.5
100.00	373.15	790.9
1000.00	298.15	884.8
1000.00	303.15	879.0
1000.00	308.15	873.2
1000.00	313.15	867.4
1000.00	318.15	861.5
1000.00	323.15	856.0
1000.00	328.15	850.2
1000.00	333.15	844.2
1000.00	338.15	838.2
1000.00	343.15	832.2
1000.00	348.15	826.0
1000.00	353.15	819.9
1000.00	363.15	805.1
1000.00	373.15	792.6
1000.00	383.15	780.0
1000.00	393.15	766.4
2000.00	298.15	885.7
2000.00	303.15	880.0
2000.00	308.15	874.2
2000.00	313.15	868.4
2000.00	318.15	862.6
2000.00	323.15	857.1
2000.00	328.15	851.3
2000.00	333.15	845.4
2000.00	338.15	839.5
2000.00	343.15	833.5
2000.00	348.15	827.4
2000.00	353.15	821.3
2000.00	363.15	806.9
2000.00	373.15	794.5
2000.00	383.15	782.1
2000.00	393.15	768.7
3000.00	298.15	886.6
3000.00	303.15	880.9
3000.00	308.15	875.2
3000.00	313.15	869.4
3000.00	318.15	863.7
3000.00	323.15	858.1
3000.00	328.15	852.5

3000.00	333.15	846.6
3000.00	338.15	840.7
3000.00	343.15	834.8
3000.00	348.15	828.8
3000.00	353.15	822.7
3000.00	363.15	808.7
3000.00	373.15	796.4
3000.00	383.15	784.1
3000.00	393.15	770.8
3340.00	298.15	886.9
3340.00	303.15	881.2
3340.00	308.15	875.5
3340.00	313.15	869.8
3340.00	318.15	864.1
3340.00	323.15	858.4
3340.00	328.15	852.9
3340.00	333.15	847.0
3340.00	338.15	841.1
3340.00	343.15	835.2
3340.00	348.15	829.3
3340.00	353.15	823.2
3340.00	363.15	809.3
3340.00	373.15	797.1
3340.00	383.15	784.8
3340.00	393.15	771.5
5000.00	298.15	888.7
5000.00	303.15	883.0
5000.00	308.15	877.4
5000.00	313.15	871.7
5000.00	318.15	866.1
5000.00	323.15	860.3
5000.00	328.15	854.7
5000.00	333.15	849.0
5000.00	338.15	843.1
5000.00	343.15	837.4
5000.00	348.15	831.5
5000.00	353.15	825.6
5000.00	363.15	812.0
5000.00	373.15	800.0
5000.00	383.15	787.9
5000.00	393.15	775.0
10000.00	298.15	892.9
10000.00	303.15	887.4
10000.00	308.15	882.0

10000.00	313.15	876.5
10000.00	318.15	871.0
10000.00	323.15	865.4
10000.00	328.15	860.0
10000.00	333.15	854.6
10000.00	338.15	848.8
10000.00	343.15	843.4
10000.00	348.15	837.7
10000.00	353.15	832.1
10000.00	363.15	819.6
10000.00	373.15	808.2
10000.00	383.15	796.6
10000.00	393.15	784.5
15000.00	298.15	896.9
15000.00	303.15	891.6
15000.00	308.15	886.3
15000.00	313.15	880.9
15000.00	318.15	875.6
15000.00	323.15	870.2
15000.00	328.15	865.0
15000.00	333.15	859.7
15000.00	338.15	854.4
15000.00	343.15	848.9
15000.00	348.15	843.4
15000.00	353.15	838.0
15000.00	363.15	826.5
15000.00	373.15	815.6
15000.00	383.15	804.6
15000.00	393.15	793.1
20000.00	298.15	900.7
20000.00	303.15	895.6
20000.00	308.15	890.4
20000.00	313.15	885.1
20000.00	318.15	880.0
20000.00	323.15	874.7
20000.00	328.15	869.6
20000.00	333.15	864.5
20000.00	338.15	859.4
20000.00	343.15	854.0
20000.00	348.15	848.8
20000.00	353.15	843.5
20000.00	363.15	833.0
20000.00	373.15	822.5
20000.00	383.15	811.9

20000.00	393.15	800.8
25000.00	298.15	904.4
25000.00	303.15	899.4
25000.00	308.15	894.3
25000.00	313.15	889.3
25000.00	318.15	884.1
25000.00	323.15	879.1
25000.00	328.15	874.0
25000.00	333.15	869.2
25000.00	338.15	863.6
25000.00	343.15	859.1
25000.00	348.15	854.0
25000.00	353.15	848.9
25000.00	363.15	839.1
25000.00	373.15	829.0
25000.00	383.15	818.7
25000.00	393.15	808.0
30000.00	298.15	908.9
30000.00	303.15	904.0
30000.00	308.15	899.2
30000.00	313.15	894.4
30000.00	318.15	889.1
30000.00	323.15	884.3
30000.00	328.15	879.4
30000.00	333.15	874.8
30000.00	338.15	869.9
30000.00	343.15	865.0
30000.00	348.15	860.1
30000.00	353.15	855.3
30000.00	363.15	844.8
30000.00	373.15	834.9
30000.00	383.15	825.0
30000.00	393.15	814.7
35000.00	298.15	913.6
35000.00	303.15	908.9
35000.00	308.15	904.2
35000.00	313.15	899.5
35000.00	318.15	894.3
35000.00	323.15	889.7
35000.00	328.15	884.9
35000.00	333.15	880.6
35000.00	338.15	875.8
35000.00	343.15	871.0
35000.00	348.15	866.3

35000.00	353.15	861.6
35000.00	363.15	850.2
35000.00	373.15	840.6
35000.00	383.15	830.9
35000.00	393.15	820.9

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Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
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
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
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tcondl:	Liquid thermal conductivity
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility