Methyl propionate

Other names:	C2H5COOCH3
	Methyl ester of propanoic acid
	Methyl propanoate
	Methyl propylate
	Methylester kyseliny propionove
	NSC 9375
	Propanoic acid, methyl ester
	Propionate de methyle
	Propionic acid, methyl ester
	UN 1248
Inchi:	InChI=1S/C4H8O2/c1-3-4(5)6-2/h3H2,1-2H3
InchiKey:	RJUFJBKOKNCXHH-UHFFFAOYSA-N
Formula:	C4H8O2
SMILES:	CCC(=O)OC
Mol. weight [g/mol]:	88.11
CAS:	554-12-1

Physical Properties

Property code	Value	Unit	Source
affp	830.20	kJ/mol	NIST Webbook
basg	799.20	kJ/mol	NIST Webbook
chl	-2246.00	kJ/mol	NIST Webbook
gf	-251.12	kJ/mol	Joback Method
hf	-370.69	kJ/mol	Joback Method
hfus	8.90	kJ/mol	Joback Method
hvap	32.30 ± 0.02	kJ/mol	NIST Webbook
hvap	35.95	kJ/mol	NIST Webbook
hvap	34.50 ± 4.20	kJ/mol	NIST Webbook
hvap	35.82 ± 0.09	kJ/mol	NIST Webbook
ie	10.30	eV	NIST Webbook
ie	10.15 ± 0.03	eV	NIST Webbook
ie	10.15 ± 0.03	eV	NIST Webbook
ie	10.15	eV	NIST Webbook
ie	10.15	eV	NIST Webbook
ie	9.90 ± 0.20	eV	NIST Webbook
log10ws	-0.14		Aqueous Solubility Prediction Method

log10ws	-0.14		Estimated Solubility Method
logp	0.569		Crippen Method
mcvol	74.660	ml/mol	McGowan Method
pc	4041.00 ± 101.32	kPa	NIST Webbook
pc	4041.00 ± 101.32	kPa	NIST Webbook
pc	4005.00 ± 40.00	kPa	NIST Webbook
pc	4004.00 ± 101.32	kPa	NIST Webbook
rhoc	312.33 ± 4.41	kg/m3	NIST Webbook
rhoc	300.44 ± 9.69	kg/m3	NIST Webbook
rhoc	300.44 ± 9.69	kg/m3	NIST Webbook
rhoc	311.89 ± 9.69	kg/m3	NIST Webbook
rinpol	615.20		NIST Webbook
rinpol	615.00		NIST Webbook
rinpol	607.00		NIST Webbook
rinpol	622.00		NIST Webbook
rinpol	627.00		NIST Webbook
rinpol	610.00		NIST Webbook
rinpol	629.00		NIST Webbook
rinpol	624.00		NIST Webbook
rinpol	625.70		NIST Webbook
rinpol	628.20		NIST Webbook
rinpol	614.00		NIST Webbook
rinpol	629.00		NIST Webbook
rinpol	618.00		NIST Webbook
rinpol	618.00		NIST Webbook
rinpol	639.00		NIST Webbook
rinpol	617.00		NIST Webbook
rinpol	612.00		NIST Webbook
rinpol	607.00		NIST Webbook
rinpol	600.00		NIST Webbook
rinpol	627.00		NIST Webbook
rinpol	611.60		NIST Webbook
rinpol	621.00		NIST Webbook
rinpol	615.00		NIST Webbook
rinpol	610.00		NIST Webbook
rinpol	617.00		NIST Webbook
rinpol	617.00		NIST Webbook
rinpol	621.00		NIST Webbook
rinpol	600.00		NIST Webbook
rinpol	621.00		NIST Webbook
rinpol	639.00		NIST Webbook
rinpol	616.00		NIST Webbook
rinpol	616.00		NIST Webbook
rinpol	621.00		NIST Webbook

rinpol	615.00	NIST Webbook
rinpol	617.00	NIST Webbook
rinpol	604.00	NIST Webbook
rinpol	611.00	NIST Webbook
rinpol	617.00	NIST Webbook
rinpol	622.00	NIST Webbook
rinpol	617.00	NIST Webbook
rinpol	621.00	NIST Webbook
rinpol	611.00	NIST Webbook
rinpol	613.00	NIST Webbook
rinpol	618.00	NIST Webbook
rinpol	611.00	NIST Webbook
rinpol	630.00	NIST Webbook
rinpol	642.60	NIST Webbook
rinpol	618.00	NIST Webbook
rinpol	626.00	NIST Webbook
rinpol	611.00	NIST Webbook
rinpol	627.00	NIST Webbook
rinpol	627.00	NIST Webbook
ripol	872.00	NIST Webbook
ripol	885.00	NIST Webbook
ripol	908.00	NIST Webbook
ripol	904.00	NIST Webbook
ripol	906.00	NIST Webbook
ripol	910.00	NIST Webbook
ripol	905.00	NIST Webbook
ripol	885.00	NIST Webbook
ripol	896.00	NIST Webbook
ripol	911.00	NIST Webbook
ripol	905.00	NIST Webbook
ripol	905.00	NIST Webbook
ripol	904.00	NIST Webbook
ripol	904.00	NIST Webbook
ripol	896.00	NIST Webbook
ripol	937.00	NIST Webbook
ripol	872.00	NIST Webbook
ripol	872.00	NIST Webbook
ripol	906.00	NIST Webbook
ripol	901.00	NIST Webbook
ripol	911.00	NIST Webbook
ripol	885.00	NIST Webbook
ripol	896.00	NIST Webbook
ripol	890.00	NIST Webbook
ripol	908.00	NIST Webbook

ripol	899.00		NIST Webbook
ripol	908.00		NIST Webbook
ripol	906.00		NIST Webbook
ripol	916.00		NIST Webbook
ripol	905.00		NIST Webbook
ripol	909.00		NIST Webbook
ripol	900.00		NIST Webbook
ripol	937.00		NIST Webbook
tb	353.00 ± 0.50	K	NIST Webbook
tb	352.70 ± 1.00	K	NIST Webbook
tb	352.85 ± 0.50	K	NIST Webbook
tb	352.80 ± 0.50	K	NIST Webbook
tb	352.80 ± 0.50	K	NIST Webbook
tb	352.85 ± 0.50	K	NIST Webbook
tb	353.70 ± 0.30	K	NIST Webbook
tb	352.15 ± 1.00	K	NIST Webbook
tb	353.03 ± 0.50	K	NIST Webbook
tb	352.95 ± 1.00	K	NIST Webbook
tb	352.00 ± 2.00	K	NIST Webbook
tb	353.00 ± 2.00	K	NIST Webbook
tb	353.15 ± 1.00	K	NIST Webbook
tb	351.15 ± 10.00	K	NIST Webbook
tb	353.15 ± 1.00	K	NIST Webbook
tb	353.65 ± 2.00	K	NIST Webbook
tb	352.47	K	Isobaric Vapor-Liquid Phase Equilibrium Measurements for Allyl Alcohol with Chloroform, Ethyl Acetate, and Methyl Propionate at 101.3 kPa
tb	352.65 ± 1.00	K	NIST Webbook
tb	352.15 ± 2.00	K	NIST Webbook
tb	352.91 ± 0.50	K	NIST Webbook
tb	352.53 ± 0.50	K	NIST Webbook
tb	352.85 ± 0.20	K	NIST Webbook
tb	352.90	K	NIST Webbook
tb	353.10	K	NIST Webbook
tb	351.65 ± 0.30	K	NIST Webbook
tb	351.65	K	Isobaric Vapor-Liquid Equilibria and Excess Properties for the Binary Systems of Methyl Esters + Heptane
tb	352.70 ± 0.60	K	NIST Webbook
tb	352.65	K	Multiphase equilibria for mixtures containing water, acetic acid, propionic acid, methyl acetate and methyl propionate

tb	352.62	K	Experimental determination of vapor liquid equilibrium for methanol + methyl propionate + 1-butyl-3-methylimidazo-lium bis(trifluoromethylsulfonyl)imide at atmospheric pressure
tc	546.48	K	Joback Method
tf	185.27	K	Aqueous Solubility Prediction Method
tf	185.65 ± 0.50	K	NIST Webbook
vc	0.283	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.49	J/mol×K	397.09	Joback Method
cpg	168.41	J/mol×K	546.48	Joback Method
cpg	162.40	J/mol×K	516.61	Joback Method
cpg	156.20	J/mol×K	486.73	Joback Method
cpg	149.81	J/mol×K	456.85	Joback Method
cpg	143.24	J/mol×K	426.97	Joback Method
cpg	129.57	J/mol×K	367.21	Joback Method
cpl	171.21	J/mol×K	298.15	NIST Webbook
cpl	174.20	J/mol×K	298.15	NIST Webbook
cpl	175.90	J/mol×K	298.38	NIST Webbook
cpl	171.20	J/mol×K	298.15	NIST Webbook
cpl	172.74	J/mol×K	298.15	NIST Webbook
cpl	174.60	J/mol×K	301.45	NIST Webbook
dvisc	0.0013870	Pa×s	233.70	Joback Method
dvisc	0.0008729	Pa×s	260.40	Joback Method
dvisc	0.0005988	Pa×s	287.11	Joback Method
dvisc	0.0004380	Pa×s	313.81	Joback Method
dvisc	0.0003364	Pa×s	340.51	Joback Method
dvisc	0.0024835	Pa×s	207.00	Joback Method
dvisc	0.0002686	Pa×s	367.21	Joback Method
hvapt	32.24	kJ/mol	352.90	NIST Webbook

pvap	101.30	kPa	352.47	Isobaric Vapor-Liquid Phase Equilibrium Measurements for Allyl Alcohol with Chloroform, Ethyl Acetate, and Methyl Propionate at 101.3 kPa
pvap	101.30	kPa	352.62	Experimental determination of vapor liquid equilibrium for methanol + methyl propionate + 1-butyl-3-methylimidazo-lium bis(trifluoromethylsulfonyl)imide at atmospheric pressure
pvap	101.30	kPa	352.65	Multiphase equilibria for mixtures containing water, acetic acid, propionic acid, methyl acetate and methyl propionate
rfi	1.36410		318.15	Thermodynamic properties of (an ester + and alkane). XVII. Experimental He and Ve values for (an alkyl propanoate + an alkane) at 318.15K
rfi	1.37421		298.15	Excess molar volumes and excess molar enthalpies for binary mixtures of 1,2-dichloropropane with methyl ethanoate, methyl propanoate, and methyl butanoate at T = 298.15K

rfi	1.37430		298.15	Improvements in the Experimentation and the Representation of Thermodynamic Properties (iso-p VLE and yE) of Alkyl Propanoate + Alkane Binaries
rfi	1.36410		318.15	Excess Properties and Isobaric Vapor-Liquid Equilibria for Binary Mixtures of Methyl Esters + tert-Butanol
rfi	1.37400		298.15	Thermodynamic study of (alkyl esters + alpha,omega-alkyl dihalides) IV: Hex and Vex for 25 binary mixtures {xC(u-1)H(2u-1)CO2CH3 + (1-x)alpha,omega-BrCH2(CH2)(v-2)CH2Br}, where u = 1 to 5, alpha = 1 and v = omega = 2 to 6
rhol	909.30	kg/m3	298.15	Densities and interfacial tensions for fatty acid methyl esters (from methyl formate to methyl heptanoate) + water demixed mixtures at atmospheric pressure conditions

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45878e+01
Coeff. B	-3.06195e+03
Coeff. C	-4.58670e+01
Temperature range (K), min.	259.99

Temperature range (K), max.	375.95

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.37412e+01
Coeff. B	-7.00860e+03
Coeff. C	-1.02625e+01
Coeff. D	7.55664e-06
Temperature range (K), min.	185.65
Temperature range (K), max.	530.60

Sources

Isothermal (vapour + liquid) equilibria for the binary systems of (carbon monoxide + methyl propionate) and (carbon monoxide + ethyl propionate):	https://www.doi.org/10.1016/j.jct.2012.11.028
Thermodynamics and limiting activity coefficients measurements for organic solutes and water in the ionic liquid 1-dodecyl-3-methylimidzolium bis(trifluoromethylsulfonyl) imide:	https://www.doi.org/10.1016/j.jct.2016.08.008
Experimental determination of vapor liquid equilibrium for methanol + methyl propionate + 1-butyl-3-methylimidazo-lium bis(trifluoromethylsulfonyl)imide at atmospheric pressure	https://www.doi.org/10.1016/j.jct.2019.01.004
Separation of water/butan-1-ol based on activity coefficients at infinite dilution in 1,3-didecyl-2-methylimidazolium dicyanamide ionic liquid.	https://www.doi.org/10.1016/j.jct.2017.10.003
Activity coefficients at infinite dilution for organic solutes and water in [illegible] lactate.	https://www.doi.org/10.1016/j.jct.2015.05.014
Thermodynamic Properties of Mixtures Containing Ionic Liquids. 8. Activity Coefficients at Infinite Dilution of Hydrocarbons, Alcohols, Esters, and Aldehydes in 1-Hexyl-3-methylimidazolium Bis(trifluoromethylsulfonyl) Imide Using Gas-Liquid Chromatography:	https://www.doi.org/10.1021/je0503554
Solubility of ethylene in methyl propionate:	https://www.doi.org/10.1016/j.fluid.2014.12.019
Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid [illegible]	https://www.doi.org/10.1016/j.jct.2012.08.016
Experimental Study of Thermodynamic Properties of Mixtures Containing Ionic Liquid 1-Ethyl-3-methylimidazolium Ethyl Sulfate Using Gas-Liquid Chromatography and Transpiration Method	https://www.doi.org/10.1021/je0602723
Separation on investigation of limiting activity coefficients in [illegible] ionic liquid in the separation processes:	https://www.doi.org/10.1016/j.fluid.2017.06.001
[illegible] 1-methylpiperidinium trifluorotris(perfluoroethyl)phosphate:	https://www.doi.org/10.1016/j.jct.2016.01.017
Solubility and Thermodynamic Modeling of Dimethyl Terephthalate in Pure Solvents and the Evaluation of the Mixing Properties of the Solutions:	https://www.doi.org/10.1021/acs.jced.9b00658
Thermodynamics and activity coefficients at infinite dilution for organic solutes and water in the ionic liquid 1-butyl-1-methylmorpholinium tricyanomethanide:	https://www.doi.org/10.1016/j.jct.2013.08.030
Thermodynamic study of (alkyl esters + alpha,omega-alkyl dihalides) IV: Hex [illegible] {xCu-1H(2u-1)CO2CH3 + (1-x)alpha,omega-BrCH2(CH2)(v-2)CH2Br}, where u = 1 to 3, and v = 2 to 6	https://www.doi.org/10.1016/j.jct.2006.05.004
Separation of binary mixtures based on limiting activity coefficients data using [illegible]	https://www.doi.org/10.1016/j.fluid.2017.12.029
Activity coefficients at infinite dilution of organic solvents and water in 1-ethyl-3-methylimidazolium dicyanamide. A literature review of hexane/hex-1-ene separation.	https://www.doi.org/10.1016/j.fluid.2016.02.004
Isobaric Vapor-Liquid Phase Equilibrium Measurements for Allyl [illegible] Ethyl Acetate, and Methyl Propionate at 101.3 kPa.	https://www.doi.org/10.1021/acs.jced.8b00908
Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid 1-(2-methoxyethyl)-1-methylpyrrolidinium trifluorotris(perfluoroethyl)phosphate:	https://www.doi.org/10.1016/j.jct.2013.01.007
Thermodynamics and selectivity of separation based on activity coefficients at infinite dilution of various solutes in 1-allyl-3-methylimidazolium bis{(trifluoromethyl)sulfonyl}imide ionic liquid	https://www.doi.org/10.1016/j.jct.2016.06.028
Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid 4-(2-methoxyethyl)-4-methylmorpholinium bis(trifluoromethylsulfonyl)-amide	https://www.doi.org/10.1016/j.jct.2011.11.021
Measurements of activity coefficients at infinite dilution for organic solutes and water in the ionic liquid [illegible] tetracyanoborate.	https://www.doi.org/10.1016/j.jct.2011.11.025
Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid 4-(3-hydroxypropyl)-4-methylmorpholinium bis(trifluoromethylsulfonyl)-amide:	https://www.doi.org/10.1016/j.jct.2015.02.024
Densities and interfacial tensions for fatty acid methyl esters (from methyl [illegible] methyl heptanoate) + water demixed mixtures at atmospheric pressure conditions.	https://www.doi.org/10.1016/j.jct.2018.02.010
NIST Webbook	http://webbook.nist.gov/cgi/cbook.cgi?ID=C554121&Units=SI
Thermodynamic study of molecular interaction-selectivity in separation processes based on limiting activity coefficients.	https://www.doi.org/10.1016/j.jct.2018.02.014
Isobaric Vapor-Liquid Equilibria and Excess Properties for the Binary Systems of Methyl Esters + Heptane:	https://www.doi.org/10.1021/je030117d

Thermodynamics and activity coefficients at infinite dilution for organic solutes in the ionic liquid 1-butyl-1-methylpyrrolidinium dicyanamide:	https://www.doi.org/10.1016/j.fluid.2018.06.013
Thermodynamic properties of (an ester + an alkane). XVII. Experimental He and Ve values for (an alkyl propanoate + an alkane) at 318.15K:	https://www.doi.org/10.1016/j.jct.2004.12.014
New ionic liquid [P4,4,4,4][NTf2] in bio-butanol extraction: on investigation of limiting activity coefficients:	https://www.doi.org/10.1016/j.fluid.2018.07.028
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Measurements of activity coefficients at infinite dilution for organic solutes and water in the ionic liquid 1-butyl-1-methylpyrrolidinium tricyanomethanide:	https://www.doi.org/10.1016/j.jct.2013.07.004
Improvements in the Experimentation and the Representation of Thermodynamic Properties (iso-p VLE and yE) of Alkyl Propanoate + Alkane Binaries:	https://www.doi.org/10.1021/je4009415
Thermodynamic Properties of Mixtures Containing Ionic Liquids. 9. Activity Coefficients at Infinite Dilution of Hydrocarbons, Alcohols, Esters, and Aldehydes in Trimethyl-butylammonium Bis(trifluoromethylsulfonyl) imide Using Gas-Liquid Chromatography and Static Method:	https://www.doi.org/10.1021/je050440b
Ammonium ionic liquids in extraction of bio-butan-1-ol from water phase using activity coefficients at infinite dilution:	https://www.doi.org/10.1016/j.fluid.2018.09.024
Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid trihexyl-tetradecyl-phosphonium tricyanomethanide:	https://www.doi.org/10.1016/j.jct.2018.01.003
Separation of binary mixtures hexane/hex-1-ene, cyclohexane/cyclohexene and ethylbenzene/styrene based on gamma infinity data measurements:	https://www.doi.org/10.1016/j.jct.2017.11.017
Activity coefficients at infinite dilution, physicochemical and thermodynamic properties of organic solutes and water in the ionic liquid ethyl-dimethyl-(2-methoxyethyl)ammonium trifluorotris-(perfluoroethyl)phosphate:	https://www.doi.org/10.1016/j.jct.2015.05.022
Bubble point pressures of binary system of methanol and methyl propionate:	https://www.doi.org/10.1016/j.fluid.2016.02.036
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid 1-(2-hydroxyethyl)-3-methylimidazolium trifluorotris(perfluoroethyl)phosphate:	https://www.doi.org/10.1016/j.jct.2013.05.008
Thermodynamics and activity coefficients at infinite dilution for organic solutes, water and diols in the ionic liquid [illegible] bis(trifluoromethylsulfonyl)imide:	https://www.doi.org/10.1016/j.jct.2014.04.024
Experimental determination and calculation of the critical curves for the binary systems of CO2 containing ketone, alkane, ester and alcohol, respectively:	https://www.doi.org/10.1016/j.fluid.2011.05.005
Multiphase equilibria of mixtures containing water, acetic acid, propionic acid, methyl acetate and methyl propionate:	https://www.doi.org/10.1016/j.fluid.2008.07.004
Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid 1-(2-methoxyethyl)-1-methylpiperidinium bis(trifluoromethylsulfonyl)-amide:	https://www.doi.org/10.1016/j.jct.2012.01.019
Vapor-Liquid Equilibrium Data of (Carbon Dioxide + Methyl Propionate) and (Carbon Dioxide + Ethyl Propionate) at Pressures from (1.00 to 12.00) MPa and Temperatures from (313.0 to 373.0) K:	https://www.doi.org/10.1021/je9001784
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Excess molar volumes and excess molar enthalpies for binary mixtures of 1,2-dichloropropane with methyl ethanoate, methyl propanoate, and methyl butanoate at T = 298.15K:	https://www.doi.org/10.1016/j.fluid.2011.01.005
Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid 1-(2-methoxyethyl)-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)-amide:	https://www.doi.org/10.1016/j.jct.2012.03.015
The use of ionic liquids for separation of binary hydrocarbons mixtures based on gamma infinity data measurements:	https://www.doi.org/10.1016/j.jct.2018.07.024
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1058
Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid 4-(2-methoxyethyl)-4-methylmorpholinium trifluorotris(perfluoroethyl)phosphate:	https://www.doi.org/10.1016/j.jct.2012.05.017
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Separation of binary mixtures hexane/hex-1-ene cyclohexane/cyclohexene and ethylbenzene/styrene based on limiting activity coefficients:	https://www.doi.org/10.1016/j.jct.2017.03.004
Low pressure carbon dioxide solubility in pure electrolyte solvents for lithium-ion batteries as a function of temperature. Measurement and prediction:	https://www.doi.org/10.1016/j.jct.2012.01.027
Excess Properties and Isobaric Vapor-Liquid Equilibria for Binary Mixtures of Methyl Esters + tert-Butanol:	https://www.doi.org/10.1021/je034290l

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid 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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume