Ethyl formate

Other names:	Aethylformiat
	Areginal
	Ethyl ester of formic acid
	Ethyl methanoate
	Ethyle (formiate d')
	Ethylester kyseliny mravenci
	Ethylformiaat
	Ethylformic ester
	Etile (formiato di)
	Formic acid, ethyl ester
	Formic ether
	HCOOC2H5
	Mrowczan etylu
	NSC 406578
	UN 1190
	methanoic acid, ethyl ester
Inchi:	InChI=1S/C3H6O2/c1-2-5-3-4/h3H,2H2,1H3
InchiKey:	WBJINCZRORDGAQ-UHFFFAOYSA-N
Formula:	C3H6O2
SMILES:	CCOC=O
Mol. weight [g/mol]:	74.08
CAS:	109-94-4

Physical Properties

Property code	Value	Unit	Source
af	0.2850		KDB
affp	799.40	kJ/mol	NIST Webbook
basg	768.40	kJ/mol	NIST Webbook
dm	2.00	debye	KDB
dvisc	0.0004000	Pa×s	Densities and Viscosities of 1-Butyl-3-methylimidazolium Tetrafluoroborate + Molecular Solvent Binary Mixtures
gf	-230.14	kJ/mol	Joback Method
hf	-398.00	kJ/mol	NIST Webbook
hf	-361.70	kJ/mol	NIST Webbook

hf	-371.50	kJ/mol	KDB
hfl	-394.20 ± 0.80	kJ/mol	NIST Webbook
hfl	-430.50	kJ/mol	NIST Webbook
hfus	7.00	kJ/mol	Joback Method
hvap	30.10 ± 0.01	kJ/mol	NIST Webbook
hvap	32.20	kJ/mol	NIST Webbook
hvap	32.50	kJ/mol	NIST Webbook
hvap	32.11	kJ/mol	NIST Webbook
ie	10.61 ± 0.01	eV	NIST Webbook
ie	10.61	eV	NIST Webbook
ie	10.61 ± 0.05	eV	NIST Webbook
ie	10.61 ± 0.05	eV	NIST Webbook
ie	10.62	eV	NIST Webbook
ie	10.61 ± 0.01	eV	NIST Webbook
log10ws	0.15		Aqueous Solubility Prediction Method
log10ws	0.15		Estimated Solubility Method
logp	0.179		Crippen Method
mcvol	60.570	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB
pc	4981.00 ± 202.65	kPa	NIST Webbook
pc	4930.00 ± 202.65	kPa	NIST Webbook
pc	4738.00 ± 101.32	kPa	NIST Webbook
pc	4737.00 ± 40.00	kPa	NIST Webbook
pc	4740.00	kPa	KDB
rhoc	323.20 ± 5.19	kg/m3	NIST Webbook
rhoc	323.20 ± 3.70	kg/m3	NIST Webbook
rhoc	314.83 ± 5.93	kg/m3	NIST Webbook
rinpol	502.00		NIST Webbook
rinpol	530.00		NIST Webbook
rinpol	495.00		NIST Webbook
rinpol	510.00		NIST Webbook
rinpol	495.00		NIST Webbook
rinpol	495.00		NIST Webbook
rinpol	487.00		NIST Webbook
rinpol	521.00		NIST Webbook
rinpol	502.00		NIST Webbook
rinpol	502.00		NIST Webbook
rinpol	521.00		NIST Webbook
rinpol	530.00		NIST Webbook
rinpol	545.00		NIST Webbook
rinpol	502.00		NIST Webbook
rinpol	501.00		NIST Webbook

rinpol	478.00	NIST Webbook
rinpol	495.00	NIST Webbook
rinpol	487.00	NIST Webbook
rinpol	545.00	NIST Webbook
rinpol	481.00	NIST Webbook
rinpol	502.00	NIST Webbook
rinpol	457.00	NIST Webbook
rinpol	501.00	NIST Webbook
rinpol	463.00	NIST Webbook
rinpol	474.00	NIST Webbook
rinpol	465.00	NIST Webbook
rinpol	469.00	NIST Webbook
rinpol	468.00	NIST Webbook
rinpol	495.00	NIST Webbook
rinpol	456.00	NIST Webbook
rinpol	487.00	NIST Webbook
rinpol	455.00	NIST Webbook
rinpol	468.00	NIST Webbook
rinpol	495.00	NIST Webbook
rinpol	481.00	NIST Webbook
rinpol	530.00	NIST Webbook
rinpol	481.00	NIST Webbook
rinpol	530.00	NIST Webbook
rinpol	502.00	NIST Webbook
rinpol	504.00	NIST Webbook
rinpol	500.00	NIST Webbook
ripol	825.00	NIST Webbook
ripol	814.00	NIST Webbook
ripol	849.10	NIST Webbook
ripol	823.00	NIST Webbook
ripol	822.00	NIST Webbook
ripol	810.00	NIST Webbook
ripol	806.00	NIST Webbook
ripol	830.00	NIST Webbook
ripol	804.00	NIST Webbook
ripol	806.00	NIST Webbook
ripol	825.00	NIST Webbook
ripol	800.00	NIST Webbook
ripol	820.00	NIST Webbook
ripol	834.00	NIST Webbook
ripol	821.00	NIST Webbook
ripol	811.00	NIST Webbook
ripol	820.00	NIST Webbook
ripol	849.10	NIST Webbook

ripol	842.00		NIST Webbook
ripol	837.00		NIST Webbook
ripol	848.00		NIST Webbook
ripol	822.00		NIST Webbook
ripol	847.00		NIST Webbook
ripol	832.00		NIST Webbook
ripol	820.00		NIST Webbook
ripol	825.00		NIST Webbook
tb	327.50	K	NIST Webbook
tb	326.65 ± 2.00	K	NIST Webbook
tb	327.47 ± 0.50	K	NIST Webbook
tb	327.10 ± 2.00	K	NIST Webbook
tb	328.00 ± 2.00	K	NIST Webbook
tb	327.50 ± 0.50	K	NIST Webbook
tb	327.45 ± 0.50	K	NIST Webbook
tb	327.20 ± 0.30	K	NIST Webbook
tb	327.45 ± 2.00	K	NIST Webbook
tb	326.55 ± 1.00	K	NIST Webbook
tb	327.30 ± 0.50	K	NIST Webbook
tb	327.35 ± 2.00	K	NIST Webbook
tb	328.15 ± 2.00	K	NIST Webbook
tb	328.05 ± 2.00	K	NIST Webbook
tb	327.50	K	KDB
tb	327.33	K	Solutions of alkyl methanoates and alkanes: Simultaneous modeling of phase equilibria and mixing properties. Estimation of behavior by UNIFAC with recalculation of parameters
tb	327.29	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
tb	327.33	K	Isobaric Vapor-Liquid Equilibrium Data and Excess Properties of Binary Systems Comprised of Alkyl Methanoates + Hexane
tb	327.32	K	Isobaric Vapor Liquid Equilibrium of Binary Mixtures of Vinyl Acetate and Ethyl Formate with Cumene at 97.3 kPa
tb	327.45 ± 0.40	K	NIST Webbook
tb	326.20	K	NIST Webbook
tb	327.70	K	NIST Webbook

tb	327.30 ± 0.50	K	NIST Webbook
tb	327.15 ± 0.30	K	NIST Webbook
tb	327.35 ± 0.20	K	NIST Webbook
tb	327.65 ± 2.00	K	NIST Webbook
tb	327.45 ± 1.00	K	NIST Webbook
tb	327.45 ± 2.00	K	NIST Webbook
tb	327.30 ± 0.40	K	NIST Webbook
tb	327.30 ± 0.50	K	NIST Webbook
tb	327.15 ± 2.00	K	NIST Webbook
tb	326.35 ± 1.00	K	NIST Webbook
tb	327.30 ± 0.20	K	NIST Webbook
tb	328.05 ± 2.00	K	NIST Webbook
tb	327.00 ± 2.00	K	NIST Webbook
tb	325.85 ± 2.00	K	NIST Webbook
tb	327.30 ± 0.50	K	NIST Webbook
tb	327.40 ± 0.60	K	NIST Webbook
tc	503.20 ± 4.00	K	NIST Webbook
tc	511.80 ± 2.00	K	NIST Webbook
tc	506.30 ± 2.00	K	NIST Webbook
tc	508.50 ± 1.00	K	NIST Webbook
tc	508.50 ± 1.00	K	NIST Webbook
tc	508.40	K	NIST Webbook
tc	508.50	K	KDB
tf	193.75 ± 0.40	K	NIST Webbook
tf	193.00 ± 2.00	K	NIST Webbook
tf	193.55 ± 0.50	K	NIST Webbook
tf	193.50	K	KDB
tf	192.75	K	Aqueous Solubility Prediction Method
tf	192.65 ± 0.30	K	NIST Webbook
vc	0.229	m3/kmol	KDB
zc	0.2567360		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	101.20	J/mol×K	339.12	Joback Method
cpg	106.21	J/mol×K	368.11	Joback Method
cpg	111.13	J/mol×K	397.11	Joback Method
cpg	115.94	J/mol×K	426.10	Joback Method
cpg	120.65	J/mol×K	455.10	Joback Method

cpg	125.25	J/mol×K	484.09	Joback Method
cpg	129.73	J/mol×K	513.09	Joback Method
cpl	144.30	J/mol×K	298.15	NIST Webbook
cpl	158.20	J/mol×K	290.00	NIST Webbook
cpl	148.10	J/mol×K	294.70	NIST Webbook
cpl	148.10	J/mol×K	294.70	NIST Webbook
dvisc	0.0003660	Pa×s	303.15	Viscosity, Density, and Refractive Index of Some (Ester + Hydrocarbon) Binary Mixtures at 303.15 K and 313.15 K
dvisc	0.0003390	Pa×s	313.15	Viscosity, Density, and Refractive Index of Some (Ester + Hydrocarbon) Binary Mixtures at 303.15 K and 313.15 K
dvisc	0.0004020	Pa×s	293.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0003810	Pa×s	298.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0003620	Pa×s	303.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0003450	Pa×s	308.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0003290	Pa×s	313.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0003140	Pa×s	318.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters

dvisc	0.0003000	Pa×s	323.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0003730	Pa×s	303.15	Physical Properties of Binary Mixtures of Ethyl Formate with Benzene, Isopropyl Benzene, Isobutyl Benzene, and Butylbenzene at (303.15, 308.15, and 313.15) K
dvisc	0.0003240	Pa×s	313.15	Physical Properties of Binary Mixtures of Ethyl Formate with Benzene, Isopropyl Benzene, Isobutyl Benzene, and Butylbenzene at (303.15, 308.15, and 313.15) K
dvisc	0.0003450	Pa×s	308.15	Physical Properties of Binary Mixtures of Ethyl Formate with Benzene, Isopropyl Benzene, Isobutyl Benzene, and Butylbenzene at (303.15, 308.15, and 313.15) K
hvapt	29.91	kJ/mol	327.50	NIST Webbook
hvapt	31.40	kJ/mol	313.00	NIST Webbook
hvapt	29.90	kJ/mol	412.50	NIST Webbook
hvapt	35.80	kJ/mol	274.50	NIST Webbook
hvapt	31.60 ± 0.10	kJ/mol	304.00	NIST Webbook
hvapt	30.90 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	29.80 ± 0.10	kJ/mol	328.00	NIST Webbook
pvap	101.32	kPa	327.33	Isobaric Vapor-Liquid Equilibrium Data and Excess Properties of Binary Systems Comprised of Alkyl Methanoates + Hexane

rfi	1.35800		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	1.35520		303.15	Excess Volumes of Binary Solutions of Methyl Formate, Ethyl Formate, Propyl Formate, and Benzyl Acetate with Bromo-, Chloro-, and Nitrobenzenes at (303.15, 308.15, and 313.15) K	
rhol	927.00	kg/m3	289.00	KDB	
rhol	923.40	kg/m3	291.15	Experimentation and thermodynamic representations of binaries containing compounds of low boiling points: Pentane and alkylmethanoates	
rhol	914.35	kg/m3	298.15	Experimentation and thermodynamic representations of binaries containing compounds of low boiling points: Pentane and alkylmethanoates	
rhol	916.60	kg/m3	293.15	Densities and Viscosities of Binary Mixtures Containing Ethyl Formate and 2-Alkanols: Friction Theory and Free Volume Theory	

rhol	876.00	kg/m3	323.15	Densities and Viscosities of Binary Mixtures Containing Ethyl Formate and 2-Alkanols: Friction Theory and Free Volume Theory	
rhol	903.60	kg/m3	303.15	Densities and Viscosities of Binary Mixtures Containing Ethyl Formate and 2-Alkanols: Friction Theory and Free Volume Theory	
rhol	897.10	kg/m3	308.15	Densities and Viscosities of Binary Mixtures Containing Ethyl Formate and 2-Alkanols: Friction Theory and Free Volume Theory	
rhol	890.50	kg/m3	313.15	Densities and Viscosities of Binary Mixtures Containing Ethyl Formate and 2-Alkanols: Friction Theory and Free Volume Theory	
rhol	883.00	kg/m3	318.15	Densities and Viscosities of Binary Mixtures Containing Ethyl Formate and 2-Alkanols: Friction Theory and Free Volume Theory	
rhol	910.10	kg/m3	298.15	Densities and Viscosities of Binary Mixtures Containing Ethyl Formate and 2-Alkanols: Friction Theory and Free Volume Theory	

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46571e+01
Coeff. B	-2.89533e+03
Coeff. C	-3.85850e+01
Temperature range (K), min.	240.08
Temperature range (K), max.	508.40

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.34086e+01
Coeff. B	-5.70647e+03
Coeff. C	-7.24275e+00
Coeff. D	5.41841e-06
Temperature range (K), min.	193.55
Temperature range (K), max.	508.40

Sources

Densities and Viscosities of Binary Mixtures Containing Ethyl Formate and 2-Alkanols: Friction Theory and Free Volume Theory:	https://www.doi.org/10.1021/je500848q
Experimentation and thermodynamic representations of binaries containing compounds of low boiling points: Pentane and alkyl methanoates:	https://www.doi.org/10.1016/j.fluid.2013.11.026
Measurement of Activity Coefficients at Infinite Dilution of Benzene, Toluene, Ethanol, Esters, Ketones, and Ethers at Various Temperatures in Water Using the Dilutor Technique:	https://www.doi.org/10.1021/je049875+
Solubility of Chlorpheniramine Maleate in Ethanol, 1-Propanol, 1-Butanol, Benzene, Ethyl Acetate, Ethyl Formate, and Butyl Acetate between 283 K and 333 K:	https://www.doi.org/10.1021/je7001682
Excess Volumes of Binary Solutions of Methyl Formate, Ethyl Formate, Propyl Formate, and Benzyl Acetate with Bromo-, Chloro-, and Nitrobenzenes at (303.15, 308.15, and 313.15) K:	https://www.doi.org/10.1021/je700150e
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Isobaric Vapor-Liquid Equilibria and Excess Quantities for Binary Mixtures of an Ethyl Ester + tert-Butanol and a New Approach to VLE Data Processing:	https://www.doi.org/10.1021/je0202073
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1055
Solubility, liquid-liquid equilibrium and critical states for the quaternary system formic acid – ethanol – ethyl formate – water at 298.15 K and 308.15 K:	https://www.doi.org/10.1016/j.fluid.2018.12.024
Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters:	https://www.doi.org/10.1021/je050001c
Isobaric Vapor-Liquid Equilibrium Data and Excess Properties of Binary Systems Comprised of Alkyl Methanoates + Hexane:	https://www.doi.org/10.1021/je060355j
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Solid Liquid Phase Equilibrium of N,N'-Piperazinebis(neopentylglycol)phosphoramidate in Selected Solvents from (T = (293.15 to 333.15) K:	https://www.doi.org/10.1021/acs.jced.7b00206
Thermodynamic study of (alkyl esters + α,ω-alkyl dihalides) V. Hex and Vex for 25 binary mixtures {xCu-1H2u-1CO2CH3 + (1-x)α,ω-ClCH2(CH2)v-2CH2Cl}, where u = 1 to 5, α = 1 and v = 2 to 6:	https://www.doi.org/10.1016/j.jct.2006.10.008
Thermodynamic study of (alkyl esters + α,ω-alkyl dihalides) HE and V E for 25 binary mixtures {xCu-1H2u-1CO2C2H5 + (1-x)α,ω-BrCH2(CH2)v-2CH2Br}, where u = 1 to 5, α = 1 and v = x = 2 to 6:	https://www.doi.org/10.1016/j.jct.2005.03.020
Solutions of alkyl methanoates and alkanes: Simultaneous modeling of phase equilibria and mixing properties. Estimation of behavior by UNIFAC with recalculation of parameters:	https://www.doi.org/10.1016/j.fluid.2015.05.031
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1055
Solution Thermodynamics of Benzotriazole in Different Pure Solvents:	https://www.doi.org/10.1021/acs.jced.7b01085
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Excess properties and isobaric vapor liquid equilibria for four binary systems of alkyl (methyl or butyl) methanoates with decane:	https://www.doi.org/10.1016/j.fluid.2009.12.003
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Viscosity, Density, and Refractive Index of Some (Ester + Hydrocarbon) Binary Mixtures at 308.15 K and 313.15 K:	https://www.doi.org/10.1021/je0400052
Orippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Densities and Viscosities of 1-Butyl-3-methylimidazolium Tetrafluoroborate + Molecular Solvent Mixtures:	https://www.doi.org/10.1021/je8001128
Solubility of Tiamulin Hydrogen Fumarate in Acetone, Acetonitrile, Ethyl Acetate, Ethyl Formate, and Butyl Acetate from (288.2 to 318.2) K:	https://www.doi.org/10.1021/je800838w
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C109944&Units=SI
Excess molar enthalpies of ethylformate and (1-propanol, 2-propanol, 1-butanol, 2-butanol, and 2-methyl-2-propanol) at T = (298.15 and 308.15) K and P = 0.4 and 10.1 MPa:	https://www.doi.org/10.1016/j.jct.2005.04.015
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The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Determination and correlation of solubilities of 1,2-bis(2-nitrophenoxy)ethane in Different Selected Solvents:	https://www.doi.org/10.1016/j.fluid.2013.09.058
Isobaric Vapor Liquid Equilibrium of Binary Mixtures of Vinyl Acetate and Ethyl Formate with Cumene at 97.3 kPa:	https://www.doi.org/10.1021/je7004402
Solubility Measurement and Thermodynamic Modeling for o-Toluenesulfonamide in 16 Solvents from T = 273.15 to 323.85 K:	https://www.doi.org/10.1021/acs.jced.9b00445

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility