Methyl formate

Other names:	Formiate de methyle
	Formic acid, methyl ester
	HCOOCH3
	METHYL ESTER FORMIC ACID
	METHYL METHANOATE
	Methanoic acid methyl ester
	Methyl ester of formic acid
	Methylester kyseliny mravenci
	Methylformiaat
	Methylformiat
	Mravencan methylnaty
	UN 1243
	methanoic acid, methyl ester
Inchi:	InChI=1S/C2H4O2/c1-4-2-3/h2H,1H3
InchiKey:	TZIHFWKZFHZASV-UHFFFAOYSA-N
Formula:	C2H4O2
SMILES:	COC=O
Mol. weight [g/mol]:	60.05
CAS:	107-31-3

Physical Properties

Property code	Value	Unit	Source
af	0.2570		KDB
affp	782.50	kJ/mol	NIST Webbook
aigt	729.26	K	KDB
basg	751.50	kJ/mol	NIST Webbook
chl	-972.61 ± 0.59	kJ/mol	NIST Webbook
dm	1.80	debye	KDB
dvisc	0.0003000	Pa×s	Densities and Viscosities of 1-Butyl-3-methylimidazolium Tetrafluoroborate + Molecular Solvent Binary Mixtures
fll	5.00	% in Air	KDB
flu	22.70	% in Air	KDB
fpo	240.93	K	KDB
gf	-297.40	kJ/mol	KDB

hf	-355.50	kJ/mol	NIST Webbook
hf	-336.90	kJ/mol	NIST Webbook
hf	-349.00	kJ/mol	NIST Webbook
hf	-350.00	kJ/mol	KDB
hf	-362.00	kJ/mol	NIST Webbook
hfl	-378.00	kJ/mol	NIST Webbook
hfl	-391.00	kJ/mol	NIST Webbook
hfl	-386.10	kJ/mol	NIST Webbook
hfl	-365.90	kJ/mol	NIST Webbook
hfus	4.41	kJ/mol	Joback Method
hvap	29.18	kJ/mol	Joback Method
ie	10.30	eV	NIST Webbook
ie	11.00	eV	NIST Webbook
ie	10.84	eV	NIST Webbook
ie	10.84	eV	NIST Webbook
ie	10.70	eV	NIST Webbook
ie	10.99	eV	NIST Webbook
ie	10.85	eV	NIST Webbook
ie	10.85 ± 0.05	eV	NIST Webbook
ie	10.81 ± 0.01	eV	NIST Webbook
ie	10.85	eV	NIST Webbook
log10ws	0.58		Aqueous Solubility Prediction Method
log10ws	0.58		Estimated Solubility Method
logp	-0.211		Crippen Method
mcvol	46.480	ml/mol	McGowan Method
nfpaf	%!d(float64=4)		KDB
nfpah	%!d(float64=2)		KDB
nfpas	%!d(float64=1)		KDB
pc	6007.50 ± 40.00	kPa	NIST Webbook
pc	6247.00 ± 202.65	kPa	NIST Webbook
pc	6004.00 ± 60.79	kPa	NIST Webbook
pc	5998.00	kPa	KDB
rhoc	349.38 ± 4.80	kg/m3	NIST Webbook
rhoc	349.38 ± 4.20	kg/m3	NIST Webbook
rinpol	386.00		NIST Webbook
rinpol	386.00		NIST Webbook
rinpol	401.10		NIST Webbook
rinpol	401.10		NIST Webbook
rinpol	386.00		NIST Webbook
rinpol	370.00		NIST Webbook
rinpol	369.00		NIST Webbook
rinpol	407.00		NIST Webbook
rinpol	407.00		NIST Webbook

rinpol	380.00		NIST Webbook
rinpol	373.00		NIST Webbook
rinpol	386.00		NIST Webbook
rinpol	370.00		NIST Webbook
rinpol	373.00		NIST Webbook
rinpol	362.00		NIST Webbook
rinpol	369.00		NIST Webbook
rinpol	377.00		NIST Webbook
rinpol	376.00		NIST Webbook
ripol	761.00		NIST Webbook
ripol	757.00		NIST Webbook
ripol	779.00		NIST Webbook
ripol	779.00		NIST Webbook
ripol	779.00		NIST Webbook
tb	304.89	K	Isobaric Vapor-Liquid Equilibium for the Binary Systems of Methyl Formate with o-Xylene, m-Xylene, p-Xylene, and Ethylbenzene at 101.33 kPa
tb	304.70	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	304.79	K	Isobaric Vapor-Liquid Equilibria and Excess Properties for the Binary Systems of Methyl Esters + Heptane
tb	304.70	K	Isobaric Vapor-Liquid Equilibrium Data and Excess Properties of Binary Systems Comprised of Alkyl Methanoates + Hexane
tb	304.80	K	KDB
tc	487.20 ± 1.00	K	NIST Webbook
tc	485.20 ± 2.00	K	NIST Webbook
tc	487.20 ± 1.00	K	NIST Webbook
tc	523.70 ± 20.00	K	NIST Webbook
tc	487.20	K	NIST Webbook
tc	487.20	K	KDB
tf	173.20 ± 2.00	K	NIST Webbook
tf	173.40	K	Aqueous Solubility Prediction Method
tf	173.40 ± 0.30	K	NIST Webbook
tf	174.00	K	KDB

vc	0.172	m3/kmol	KDB
zc	0.2546780		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	73.11	J/mol×K	316.24	Joback Method
cpg	89.09	J/mol×K	460.87	Joback Method
cpg	85.96	J/mol×K	431.94	Joback Method
cpg	82.80	J/mol×K	403.02	Joback Method
cpg	79.59	J/mol×K	374.09	Joback Method
cpg	76.36	J/mol×K	345.17	Joback Method
cpg	92.17	J/mol×K	489.79	Joback Method
cpl	130.00	J/mol×K	298.00	NIST Webbook
cpl	121.30	J/mol×K	288.00	NIST Webbook
cpl	119.70	J/mol×K	298.15	NIST Webbook
cpl	95.50	J/mol×K	297.00	NIST Webbook
cpl	120.57	J/mol×K	298.75	NIST Webbook
dvisc	0.0018060	Pa×s	176.53	Joback Method
dvisc	0.0010556	Pa×s	199.81	Joback Method
dvisc	0.0006902	Pa×s	223.10	Joback Method
dvisc	0.0004890	Pa×s	246.38	Joback Method
dvisc	0.0003677	Pa×s	269.67	Joback Method
dvisc	0.0002358	Pa×s	316.24	Joback Method
dvisc	0.0002893	Pa×s	292.95	Joback Method
hvapt	28.20	kJ/mol	305.10	KDB
hvapt	27.92	kJ/mol	304.70	NIST Webbook
hvapt	29.60	kJ/mol	292.00	NIST Webbook
hvapt	28.70 ± 0.10	kJ/mol	293.00	NIST Webbook
hvapt	27.90 ± 0.10	kJ/mol	305.00	NIST Webbook
hvapt	27.40 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	30.10	kJ/mol	283.00	NIST Webbook
hvapt	28.40	kJ/mol	374.00	NIST Webbook

pvap	114.88	kPa	308.15	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	101.32	kPa	304.70	Isobaric Vapor-Liquid Equilibrium Data and Excess Properties of Binary Systems Comprised of Alkyl Methanoates + Hexane	
rfi	1.34359		293.10	Vapor-Liquid Equilibrium for Methoxymethane + Methyl Formate, Methoxymethane + Hexane, and Methyl Formate + Methanol	
rfi	1.34020		299.15	Excess Properties and Isobaric Vapor-Liquid Equilibria for Binary Mixtures of Methyl Esters + tert-Butanol	
rfi	1.34110		298.15	Mixing thermodynamic properties of ester-containing solutions: A study on the ternary (methyl alkanoate (pentanoate and methanoate) + methanol) and the corresponding binaries. New contributions to the (ester + ester) interactions	

rfi	1.34150		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
rfi	1.33930		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	974.00	kg/m3	293.00	KDB
rhol	960.85	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
rhol	980.82	kg/m3	288.15	Isobaric vapor-liquid equilibria for binary mixtures from methyl methanoate, dimethoxymethane and dimethyl carbonate at 101.33 kPa
rhol	966.54	kg/m3	298.15	Experimentation and thermodynamic representations of binaries containing compounds of low boiling points: Pentane and alkylmethanoates

rhol	977.21	kg/m3	291.15	Experimentation and thermodynamic representations of binaries containing compounds of low boiling points: Pentane and alkylmethanoates

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42260e+01
Coeff. B	-2.62106e+03
Coeff. C	-3.61910e+01
Temperature range (K), min.	224.24
Temperature range (K), max.	487.20

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.57116e+01
Coeff. B	-5.45175e+03
Coeff. C	-7.66441e+00
Coeff. D	6.72918e-06
Temperature range (K), min.	174.15
Temperature range (K), max.	487.20

Sources

Densities and interfacial tensions for fatty acid methyl esters (from methyl formate to methyl heptanoate) + water demixed mixtures at atmospheric pressure conditions:	https://www.doi.org/10.1016/j.jct.2018.02.010
Excess Properties and Isobaric Vapor-Liquid Equilibria for Binary Mixtures of Methyl Esters + tert-Butanol:	https://www.doi.org/10.1021/je034290l
Isobaric Vapor-Liquid Equilibrium for the Binary Systems of Methyl Formate with o-Xylene, m-Xylene, p-Xylene, and Ethylbenzene at 101.33 kPa:	https://www.doi.org/10.1021/je200974r
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 = x = 2 to 6:	https://www.doi.org/10.1016/j.jct.2006.10.008
Solubilities of Betulin in Fourteen Organic Solvents at Different Temperatures:	https://www.doi.org/10.1021/je700069g
Isobaric vapor-liquid equilibria for binary mixtures from methyl methanoate, dimethoxymethane and dimethyl carbonate at 101.33 kPa:	https://www.doi.org/10.1016/j.fluid.2015.03.049

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
Vapor-Liquid Equilibrium for Methoxymethane + Methyl Formate, Methoxymethane + Hexane, and Methyl Formate + Methanol:	https://www.doi.org/10.1021/je200140m
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+
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Thermodynamic study of (alkyl esters + alpha,omega-alkyl dihalides) IV: Hex and Vex for 25 binary mixtures {xCu(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:	https://www.doi.org/10.1016/j.jct.2006.05.004
Excess molar enthalpies of methylformate + (1-propanol, 2-propanol, 1-butanol, 2-butanol and 1-pentanol) at T = 298.15 K, p = (5.0, 10.0) MPa and methylformate + 1-propanol at T = 333.15 K, p = 10.0 MPa:	https://www.doi.org/10.1016/j.tca.2005.11.041
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C107313&Units=SI
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
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
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1053
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Experiments and Correlations of the Vapor Liquid Equilibria for Carbon Monoxide + Propionic Acid and Carbon Monoxide + Methyl Formate Systems:	https://www.doi.org/10.1021/je3001969
Isobaric Vapor-Liquid Equilibria and Excess Properties for the Binary Systems of Methyl Esters + Heptane:	https://www.doi.org/10.1021/je030117d
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Mixing thermodynamic properties of ester-containing solutions: A study on the ternary (methyl alkanoate (pentanoate and methanoate) + methanol) and the corresponding binaries [illegible]	https://www.doi.org/10.1016/j.jct.2015.02.019
Measurement of Activity Coefficients of Solutes at Infinite Dilution in (Dimethyl [illegible]	https://www.doi.org/10.1021/je030122h
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:	https://www.doi.org/10.1021/je0255628
Solubility of Carbon Monoxide and Hydrogen in Methanol and Methyl Formate: 298–373 K and 0.1–3.3 MPa:	https://www.doi.org/10.1021/acs.jced.9b00676
Isobaric Vapor-Liquid Equilibrium Data and Excess Properties of Binary Systems Comprised of Alkyl Methanoates + Hexane:	https://www.doi.org/10.1021/je060355j
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1053.mol
Excess properties and isobaric vapor liquid equilibria for four binary systems of alkyl (methyl to butyl) methanoates with decane:	https://www.doi.org/10.1016/j.fluid.2009.12.003
Densities and Viscosities of 1-Butyl-3-methylimidazolium Tetrafluoroborate + Molecular Solvent Binary Mixtures:	https://www.doi.org/10.1021/je8001128

Legend

af:	Acentric Factor
affp:	Proton affinity
aigt:	Autoignition Temperature
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
fll:	Lower Flammability Limit
flu:	Upper Flammability Limit
fpo:	Flash Point (Open Cup Method)
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
nfpas:	NFPA Safety 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