Formic acid, propyl ester

Other names:	Formiate de propyle
	HCOOCH2CH2CH3
	PROPYL ESTER FORMIC ACID
	Propyl ester of formic acid
	Propyl formate
	Propyl methanoate
	Propylester kyseliny mravenci
	UN 1281
	methanoic acid, propyl ester
	n-Propyl formate
Inchi:	InChI=1S/C4H8O2/c1-2-3-6-4-5/h4H,2-3H2,1H3
InchiKey:	KFNNIILCVOLYIR-UHFFFAOYSA-N
Formula:	C4H8O2
SMILES:	CCCOC=O
Mol. weight [g/mol]:	88.11
CAS:	110-74-7

Physical Properties

Property code	Value	Unit	Source
af	0.3140		KDB
affp	804.90	kJ/mol	NIST Webbook
basg	773.90	kJ/mol	NIST Webbook
chs	-2217.00 ± 42.00	kJ/mol	NIST Webbook
dm	1.90	debye	KDB
gf	-221.72	kJ/mol	Joback Method
hf	-343.69	kJ/mol	Joback Method
hfs	-500.00 ± 42.00	kJ/mol	NIST Webbook
hfus	9.59	kJ/mol	Joback Method
hvap	32.50 ± 0.04	kJ/mol	NIST Webbook
hvap	37.61	kJ/mol	NIST Webbook
hvap	37.50 ± 0.10	kJ/mol	NIST Webbook
ie	10.54 ± 0.01	eV	NIST Webbook
ie	10.54 ± 0.05	eV	NIST Webbook
ie	10.30 ± 0.20	eV	NIST Webbook
ie	10.62	eV	NIST Webbook
ie	10.50	eV	NIST Webbook
ie	10.50 ± 0.05	eV	NIST Webbook

log10ws	-0.49		Aqueous Solubility Prediction Method
log10ws	-0.49		Estimated Solubility Method
logp	0.569		Crippen Method
mcvol	74.660	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB
pc	4060.00	kPa	KDB
pc	4061.00 ± 60.79	kPa	NIST Webbook
pc	4330.00 ± 303.98	kPa	NIST Webbook
pc	4061.00 ± 40.00	kPa	NIST Webbook
rhoc	304.84 ± 5.29	kg/m3	NIST Webbook
rhoc	309.34 ± 5.29	kg/m3	NIST Webbook
rhoc	309.51 ± 4.41	kg/m3	NIST Webbook
rinpol	602.00		NIST Webbook
rinpol	559.00		NIST Webbook
rinpol	564.00		NIST Webbook
rinpol	602.00		NIST Webbook
rinpol	603.00		NIST Webbook
rinpol	603.00		NIST Webbook
rinpol	606.00		NIST Webbook
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rinpol	602.00		NIST Webbook
rinpol	592.00		NIST Webbook
rinpol	570.00		NIST Webbook
rinpol	574.00		NIST Webbook
rinpol	559.00		NIST Webbook
rinpol	602.00		NIST Webbook
rinpol	570.00		NIST Webbook
rinpol	576.00		NIST Webbook
rinpol	564.00		NIST Webbook
rinpol	572.00		NIST Webbook
rinpol	602.00		NIST Webbook
ripol	892.00		NIST Webbook
ripol	916.00		NIST Webbook
ripol	907.00		NIST Webbook
ripol	892.00		NIST Webbook
tb	354.40 ± 0.70	K	NIST Webbook
tb	354.00 ± 1.00	K	NIST Webbook

tb	354.05 ± 0.50	K	NIST Webbook
tb	354.40 ± 0.30	K	NIST Webbook
tb	354.10 ± 1.00	K	NIST Webbook
tb	353.95 ± 1.00	K	NIST Webbook
tb	354.05 ± 0.50	K	NIST Webbook
tb	354.15 ± 2.00	K	NIST Webbook
tb	354.10 ± 0.40	K	NIST Webbook
tb	354.00 ± 0.50	K	NIST Webbook
tb	354.00 ± 0.50	K	NIST Webbook
tb	354.00 ± 0.10	K	NIST Webbook
tb	354.05 ± 0.20	K	NIST Webbook
tb	354.00	K	NIST Webbook
tb	354.50	K	NIST Webbook
tb	353.92	K	Isobaric Vapor-Liquid Equilibrium Data and Excess Properties of Binary Systems Comprised of Alkyl Methanoates + Hexane
tb	354.00	K	KDB
tb	354.00 ± 2.00	K	NIST Webbook
tb	353.92	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	354.15 ± 2.00	K	NIST Webbook
tc	533.70 ± 4.00	K	NIST Webbook
tc	534.00 ± 4.00	K	NIST Webbook
tc	538.00 ± 1.00	K	NIST Webbook
tc	538.00	K	NIST Webbook
tc	538.00	K	KDB
tc	538.00 ± 1.00	K	NIST Webbook
tf	180.30 ± 0.40	K	NIST Webbook
tf	180.20	K	Aqueous Solubility Prediction Method
tf	180.20	K	KDB
vc	0.285	m3/kmol	KDB
zc	0.2586740		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	169.38	J/mol×K	535.90	Joback Method
cpg	157.65	J/mol×K	477.93	Joback Method
cpg	151.51	J/mol×K	448.95	Joback Method
cpg	145.20	J/mol×K	419.97	Joback Method
cpg	138.73	J/mol×K	390.98	Joback Method
cpg	132.08	J/mol×K	362.00	Joback Method
cpg	163.60	J/mol×K	506.91	Joback Method
cpl	171.42	J/mol×K	298.15	NIST Webbook
cpl	172.07	J/mol×K	298.15	NIST Webbook
cpl	172.10	J/mol×K	298.15	NIST Webbook
dvisc	0.0004770	Pa×s	303.15	Density and Viscosity of Propyl Formate + Aromatic Hydrocarbons at T = (303.15, 308.15, and 313.15) K
dvisc	0.0004560	Pa×s	308.15	Density and Viscosity of Propyl Formate + Aromatic Hydrocarbons at T = (303.15, 308.15, and 313.15) K
dvisc	0.0004310	Pa×s	313.15	Density and Viscosity of Propyl Formate + Aromatic Hydrocarbons at T = (303.15, 308.15, and 313.15) K
hvapt	36.80	kJ/mol	292.50	NIST Webbook
hvapt	35.80 ± 0.10	kJ/mol	326.00	NIST Webbook
hvapt	35.40 ± 0.10	kJ/mol	331.00	NIST Webbook
hvapt	34.40 ± 0.10	kJ/mol	344.00	NIST Webbook
hvapt	33.80 ± 0.10	kJ/mol	351.00	NIST Webbook
hvapt	33.50 ± 0.10	kJ/mol	355.00	NIST Webbook
hvapt	32.90 ± 0.10	kJ/mol	363.00	NIST Webbook
hvapt	33.61	kJ/mol	354.00	NIST Webbook
hvapt	35.30	kJ/mol	327.50	NIST Webbook
hvapt	32.70	kJ/mol	436.00	NIST Webbook
hvapt	35.60	kJ/mol	327.00	NIST Webbook
hvapt	36.50 ± 0.10	kJ/mol	313.00	NIST Webbook

pvap	101.32	kPa	353.92	Isobaric Vapor-Liquid Equilibrium Data and Excess Properties of Binary Systems Comprised of Alkyl Methanoates + Hexane	
rfi	1.37260		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	
rfi	1.37180		303.15	Correlation and Prediction of Excess Quantities and Vapor-Liquid Equilibria of Alkyl Esters + tert-Butyl Alcohol: Experimental Data for Propyl Esters + tert-Butyl Alcohol	
rhol	899.86	kg/m3	298.15	Experimentation and thermodynamic representations of binaries containing compounds of low boiling points: Pentane and alkylmethanoates	
rhol	907.97	kg/m3	291.15	Experimentation and thermodynamic representations of binaries containing compounds of low boiling points: Pentane and alkylmethanoates	
rhol	911.00	kg/m3	289.00	KDB	

rhol	899.81	kg/m3	298.15	Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) VII. HE m and VE m for 20 binary mixtures {xCu 1H2u 1CO2C3H7 + (1 x)a,x-ClCH2(CH2)v 2CH2Cl}, where u = 1 to 4, a = 1 and v = x = 2 to 6. An analysis of behavior using the COSMO-RS methodology

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41082e+01
Coeff. B	-2.75112e+03
Coeff. C	-6.42010e+01
Temperature range (K), min.	263.26
Temperature range (K), max.	376.94

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.34798e+01
Coeff. B	-6.18307e+03
Coeff. C	-7.14597e+00
Coeff. D	4.28442e-06
Temperature range (K), min.	180.25
Temperature range (K), max.	538.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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

Experimentation and thermodynamic representations of binaries containing compounds of low boiling points: Pentane and alkylmethanoates:	https://www.doi.org/10.1016/j.fluid.2013.11.026
Correlation and Prediction of Excess Quantities and Vapor-Liquid Equilibria of Alkyl Esters + tert-Butyl Alcohol: Experimental Data for Propyl Esters + tert-Butyl Alcohol:	https://www.doi.org/10.1021/je060003c
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1060
Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) VII. HE m and VE m for 20 binary mixtures {xCu 1H2u 1COOC3H7 + (1 x)a,x ClCH2(CH2)v 2CH2Cl}, where u = 1 to 4, a = 1 and v = x = 2 to 6: An analysis of behavior using the COSMO-RS methodology:	https://www.doi.org/10.1016/j.jct.2008.10.007
Isobaric Vapor-Liquid Equilibrium Data and Excess Properties of Binary Systems Comprised of Alkyl Methanoates + Hexane:	https://www.doi.org/10.1021/je060355j
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110747&Units=SI
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) V. Hex and Vex for 25 binary mixtures {xCu 1H2u 1COOCH3 + (1 x)a,x ClCH2(CH2)v 2CH2Cl}, where u ... Estimation of behavior by UNIFAC with recalculation of parameters:	https://www.doi.org/10.1016/j.jct.2006.10.008
Solutions of alkyl methanoates and alkanes: Simultaneous modeling of phase equilibria and mixing properties,	https://www.doi.org/10.1016/j.fluid.2015.05.031
Density and Viscosity of Propyl Formate + Aromatic Hydrocarbons at T = (303.15, 308.15, and 313.15) K:	https://www.doi.org/10.1021/je901071x
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
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:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1060

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid 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
hfs:	Solid 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