

Propanoic acid, 2-methyl-

Other names:	.alpha.-methylpropionic acid 2-METHYL-PROPANOIC ACID 2-Methylpropanoic acid 2-Methylpropionic acid 2-Propanecarboxylic acid ALPHA-METHYLPROPIONIC ACID Acetic acid, dimethyl- Cenex RP b2 Dimethylacetic acid Isobutanoic acid Isobutyric acid Isopropylformic acid Kyselina isomaseľna Methylpropanoic acid Methylpropionic acid NSC 62780 Propionic acid, 2-methyl- Tenox IBP 2 UN 2529 i-Butyric acid iso-C3H7COOH «alpha»-Methylpropanoic acid «alpha»-Methylpropionic acid Â«alphaÂ»-Methylpropanoic acid Â«alphaÂ»-Methylpropionic acid
Inchi:	InChI=1S/C4H8O2/c1-3(2)4(5)6/h3H,1-2H3,(H,5,6)
InchiKey:	KQNPFQTWMSNSAP-UHFFFAOYSA-N
Formula:	C4H8O2
SMILES:	CC(C)C(=O)O
Mol. weight [g/mol]:	88.11
CAS:	79-31-2

Physical Properties

Property code	Value	Unit	Source
af	0.6230		KDB
dm	1.30	debye	KDB

gf	-285.38	kJ/mol	Joback Method
hf	-484.20	kJ/mol	KDB
hfus	8.28	kJ/mol	Joback Method
hvap	55.50 ± 0.30	kJ/mol	NIST Webbook
hvap	53.00	kJ/mol	NIST Webbook
hvap	53.00 ± 4.00	kJ/mol	NIST Webbook
hvap	53.40 ± 3.00	kJ/mol	NIST Webbook
hvap	56.30	kJ/mol	NIST Webbook
ie	10.33	eV	NIST Webbook
ie	10.30	eV	NIST Webbook
ie	10.02 ± 0.05	eV	NIST Webbook
ie	10.33 ± 0.03	eV	NIST Webbook
ie	10.24 ± 0.12	eV	NIST Webbook
ie	10.12	eV	NIST Webbook
ie	10.33 ± 0.01	eV	NIST Webbook
log10ws	0.28		Aqueous Solubility Prediction Method
logp	0.727		Crippen Method
mcvol	74.660	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=1)		KDB
pc	3700.00	kPa	KDB
pc	3700.00 ± 25.00	kPa	NIST Webbook
rinpol	758.00		NIST Webbook
rinpol	753.00		NIST Webbook
rinpol	741.00		NIST Webbook
rinpol	790.00		NIST Webbook
rinpol	758.00		NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	731.00		NIST Webbook
rinpol	731.00		NIST Webbook
rinpol	758.00		NIST Webbook
rinpol	723.00		NIST Webbook
rinpol	753.00		NIST Webbook
rinpol	796.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	739.00		NIST Webbook
rinpol	741.00		NIST Webbook
rinpol	780.00		NIST Webbook
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rinpol	797.00	NIST Webbook
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rinpol	758.00	NIST Webbook
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rinpol	753.00	NIST Webbook
rinpol	758.00	NIST Webbook
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rinpol	774.00	NIST Webbook
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ripol	1574.00		NIST Webbook
ripol	1555.00		NIST Webbook
ripol	1578.00		NIST Webbook
ripol	1565.00		NIST Webbook
tb	427.60	K	KDB
tc	605.00	K	KDB
tc	605.00 ± 1.50	K	NIST Webbook
tc	609.40 ± 6.00	K	NIST Webbook

tf	227.05 ± 0.20	K	NIST Webbook
tf	227.15 ± 0.40	K	NIST Webbook
tf	225.25 ± 0.40	K	NIST Webbook
tf	228.15 ± 2.00	K	NIST Webbook
tf	227.00 ± 2.00	K	NIST Webbook
tf	227.05 ± 0.50	K	NIST Webbook
tf	227.20 ± 0.60	K	NIST Webbook
tf	226.90	K	Aqueous Solubility Prediction Method
tf	227.00	K	KDB
vc	0.292	m3/kmol	KDB
zc	0.2147790		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	146.25	J/mol×K	436.53	Joback Method
cpg	159.59	J/mol×K	495.77	Joback Method
cpg	165.85	J/mol×K	525.39	Joback Method
cpg	177.58	J/mol×K	584.64	Joback Method
cpg	183.06	J/mol×K	614.26	Joback Method
cpg	171.84	J/mol×K	555.02	Joback Method
cpg	153.06	J/mol×K	466.15	Joback Method
cpl	181.70	J/mol×K	298.15	NIST Webbook
cpl	173.00	J/mol×K	298.15	NIST Webbook
cpl	171.10	J/mol×K	298.00	NIST Webbook
dvisc	0.0004566	Pa×s	402.21	Joback Method
dvisc	0.0146308	Pa×s	264.91	Joback Method
dvisc	0.0663519	Pa×s	230.59	Joback Method
dvisc	0.0045636	Pa×s	299.24	Joback Method
dvisc	0.0018091	Pa×s	333.56	Joback Method
dvisc	0.0008524	Pa×s	367.88	Joback Method
dvisc	0.0002698	Pa×s	436.53	Joback Method
hvapt	50.50	kJ/mol	400.50	NIST Webbook
hvapt	55.80 ± 0.30	kJ/mol	293.00	NIST Webbook
hvapt	51.60	kJ/mol	394.50	NIST Webbook
hvapt	45.40	kJ/mol	495.00	NIST Webbook
hvapt	50.90	kJ/mol	358.00	NIST Webbook
hvapt	53.00 ± 3.00	kJ/mol	235.50	NIST Webbook

pvap	19.58	kPa	382.14	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	95.10	kPa	424.86	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	90.07	kPa	423.36	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	79.99	kPa	419.77	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	69.92	kPa	415.51	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid

pvap	59.85	kPa	410.75	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	49.79	kPa	405.44	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	39.72	kPa	399.43	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	29.65	kPa	391.77	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
pvap	100.59	kPa	426.16	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid

pvap	14.55	kPa	375.21	Subatmospheric Vapor Pressure Curves for Propionic Acid, Butyric Acid, Isobutyric Acid, Valeric Acid, Isovaleric Acid, Hexanoic Acid, and Heptanoic Acid
rfi	1.39330		293.15	Vapour liquid equilibrium of carboxylic acid systems: Propionic acid + valeric acid and isobutyric acid + valeric acid
rfi	1.39310		293.15	Vapour-liquid equilibrium of propionic acid + caproic acid, isobutyric acid + caproic acid, valeric acid + caproic acid and caproic acid + enanthoic acid binary mixtures
rfi	1.38930		303.15	Liquid liquid equilibria measurements of ternary systems (acetonitrile + a carboxylic acid + dodecane) at 303.15 K
rfi	1.38930		303.15	Phase equilibria measurements of ternary mixtures (sulfolane + a carboxylic acid + pentane) at 303.15 K
rfi	1.39130		303.15	(Liquid + liquid) equilibria measurements for ternary systems (sulfolane + a carboxylic acid + n-heptane) at T = 303.15 K and at 0.1 MPa
rhoI	941.63	kg/m3	298.20	Phase equilibria of (water + propionic acid or butyric acid + 2-methoxy-2-methylpropane) ternary systems at 298.2 K and 323.2 K

rhoI	968.00	kg/m3	293.00	KDB
rhoI	941.63	kg/m3	298.15	Tie-Line Data for Aqueous Mixtures of Butyric Acid with Diisopropyl Ether at Various Temperatures
rhoI	927.96	kg/m3	313.15	Density, speed of sound, and refractive index measurements for the binary systems (butanoic acid + propanoic acid, or 2-methyl-propanoic acid) at T = (293.15 to 313.15) K
rhoI	938.12	kg/m3	303.15	Density, speed of sound, and refractive index measurements for the binary systems (butanoic acid + propanoic acid, or 2-methyl-propanoic acid) at T = (293.15 to 313.15) K
rhoI	943.19	kg/m3	298.15	Density, speed of sound, and refractive index measurements for the binary systems (butanoic acid + propanoic acid, or 2-methyl-propanoic acid) at T = (293.15 to 313.15) K
rhoI	948.23	kg/m3	293.15	Density, speed of sound, and refractive index measurements for the binary systems (butanoic acid + propanoic acid, or 2-methyl-propanoic acid) at T = (293.15 to 313.15) K

rhoI	933.05	kg/m3	308.15	Density, speed of sound, and refractive index measurements for the binary systems (butanoic acid + propanoic acid, or 2-methyl-propanoic acid) at T = (293.15 to 313.15) K
speedsI	1100.20	m/s	295.15	Density, Speed of Sound, and Refractive Index Measurements for the Binary Mixture (1, 4-Dioxane + Isobutyric Acid) at T = (295.15, 298.15, 301.15, 304.15, 307.15, 310.15, and 313.15) K
speedsI	1086.00	m/s	298.15	Density, Speed of Sound, and Refractive Index Measurements for the Binary Mixture (1, 4-Dioxane + Isobutyric Acid) at T = (295.15, 298.15, 301.15, 304.15, 307.15, 310.15, and 313.15) K
speedsI	1072.10	m/s	301.15	Density, Speed of Sound, and Refractive Index Measurements for the Binary Mixture (1, 4-Dioxane + Isobutyric Acid) at T = (295.15, 298.15, 301.15, 304.15, 307.15, 310.15, and 313.15) K
speedsI	1058.20	m/s	304.15	Density, Speed of Sound, and Refractive Index Measurements for the Binary Mixture (1, 4-Dioxane + Isobutyric Acid) at T = (295.15, 298.15, 301.15, 304.15, 307.15, 310.15, and 313.15) K

speedsl	1015.20	m/s	313.15	Density, Speed of Sound, and Refractive Index Measurements for the Binary Mixture (1, 4-Dioxane + Isobutyric Acid) at T = (295.15, 298.15, 301.15, 304.15, 307.15, 310.15, and 313.15) K
speedsl	1030.80	m/s	310.15	Density, Speed of Sound, and Refractive Index Measurements for the Binary Mixture (1, 4-Dioxane + Isobutyric Acid) at T = (295.15, 298.15, 301.15, 304.15, 307.15, 310.15, and 313.15) K
speedsl	1043.40	m/s	307.15	Density, Speed of Sound, and Refractive Index Measurements for the Binary Mixture (1, 4-Dioxane + Isobutyric Acid) at T = (295.15, 298.15, 301.15, 304.15, 307.15, 310.15, and 313.15) K

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.55638e+01
Coeff. B	-3.91998e+03
Coeff. C	-6.88650e+01
Temperature range (K), min.	325.47
Temperature range (K), max.	451.21

Information

Value

Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	2.66544e+01
Coeff. B	-6.77334e+03
Coeff. C	-8.78498e-01
Coeff. D	-4.52289e-06
Temperature range (K), min.	227.15
Temperature range (K), max.	609.15

Sources

Phase equilibria of (water + propionic acid or butyric acid + 2-methoxy-2-methylpropane) ternary systems at 298.15 K
 Phase equilibria (acetone + a carboxylic acid + dodecane) at 303.15 K
 Liquid-liquid equilibrium for the system of ionic liquid [BMIm][HSO₄] catalysed KDB
 Butyl isobutyrate formation:

<https://www.doi.org/10.1016/j.fluid.2015.06.003>

<https://www.doi.org/10.1016/j.fluid.2014.12.013>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

<https://www.doi.org/10.1016/j.jct.2018.03.015>

<https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=933>

Chemical Equilibrium and Critical Phenomena: Solubility of Indium Oxide in Sulfuric Acid + Water Near the Consolute Point:
 Joback Method:

<https://www.doi.org/10.1021/je8008599>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C79312&Units=SI>

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

Resistivity viscosity relationship in liquid liquid critical mixtures with density, speed of sound, and refractive index measurements for the binary systems (butane + 2-propanoic acid, or 2-methyl-propanoic acid) at T = 298.15 K
 Density, Speed of Sound, and Refractive Index Measurements for the Binary Systems (1,4-Dioxane + Propionic Acid) at T = (295.15, 298.15, 301.15, 304.15, 307.15, 310.15, and 313.15) K
 Curves for Propionic Acid, Butyric Acid, and Valeric Acid on the Liquid-Liquid Equilibrium of Water + Carboxylic Acid + (1-Methylethyl)-benzene System at Several Temperatures
 Vapour-liquid equilibrium of propionic acid + caproic acid, isobutyric acid + caproic acid, and propionic acid + valeric acid systems
 Aqueous Solubility of Carboxylic Acids
 Tie-Line Data for Aqueous Mixtures of Butyric Acid with Diisopropyl Ether at Various Temperatures:

<https://www.doi.org/10.1016/j.fluid.2006.10.027>

<https://www.doi.org/10.1016/j.jct.2012.07.019>

<https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=933>

<https://www.doi.org/10.1016/j.jct.2015.12.019>

<https://www.doi.org/10.1021/je5010643>

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<https://www.doi.org/10.1016/j.fluid.2015.06.029>

<https://www.doi.org/10.1021/je034180e>

<https://www.doi.org/10.1021/je200083a>

<http://link.springer.com/article/10.1007/BF02311772>

<https://www.doi.org/10.1016/j.fluid.2014.04.026>

<https://www.doi.org/10.1016/j.fluid.2005.08.006>

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

<https://www.doi.org/10.1021/acs.jced.5b00527>

Legend

af: Acentric Factor
 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
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
rhof:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility

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