

Isopropyl acetate

Other names:

1-Methylethyl acetate
1-methylethyl ethanoate
2-Acetoxypropane
2-Propyl acetate
Acetate d'isopropyle
Acetic acid, 1-methylethyl ester
Acetic acid, 2-propyl ester
Acetic acid, isopropyl ester
CH3COOCH(CH3)2
Isopropile(acetato di)
Isopropyl (acetate d')
Isopropyl ester of acetic acid
Isopropyl ethanoate
Isopropylacetaat
Isopropylacetat
Isopropylester kyseliny octove
NSC 9295
UN 1220
ethanoic acid, isopropyl ester
sec-Propyl acetate

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

CAS:

1-Methylethyl acetate
1-methylethyl ethanoate
2-Acetoxypropane
2-Propyl acetate
Acetate d'isopropyle
Acetic acid, 1-methylethyl ester
Acetic acid, 2-propyl ester
Acetic acid, isopropyl ester
CH3COOCH(CH3)2
Isopropile(acetato di)
Isopropyl (acetate d')
Isopropyl ester of acetic acid
Isopropyl ethanoate
Isopropylacetaat
Isopropylacetat
Isopropylester kyseliny octove
NSC 9295
UN 1220
ethanoic acid, isopropyl ester
sec-Propyl acetate

InChI=1S/C5H10O2/c1-4(2)7-5(3)6/h4H,1-3H3

JMMWKPVZQRWMSS-UHFFFAOYSA-N

C5H10O2

CC(=O)OC(C)C

102.13

108-21-4

Physical Properties

Property code	Value	Unit	Source
affp	836.60	kJ/mol	NIST Webbook
basg	805.60	kJ/mol	NIST Webbook
chl	-2879.00	kJ/mol	NIST Webbook
chl	-2869.80 ± 4.10	kJ/mol	NIST Webbook
gf	-245.14	kJ/mol	Joback Method
hf	-489.70 ± 3.70	kJ/mol	NIST Webbook
hfl	-526.90 ± 3.70	kJ/mol	NIST Webbook
hfus	7.97	kJ/mol	Joback Method

hvap	33.00	kJ/mol	NIST Webbook
hvap	37.20 ± 0.20	kJ/mol	NIST Webbook
hvap	37.20 ± 0.20	kJ/mol	NIST Webbook
hvap	37.00	kJ/mol	NIST Webbook
ie	9.95 ± 0.05	eV	NIST Webbook
ie	9.99 ± 0.03	eV	NIST Webbook
ie	9.99 ± 0.03	eV	NIST Webbook
ie	10.08	eV	NIST Webbook
log10ws	-0.55		Aqueous Solubility Prediction Method
log10ws	-0.55		Estimated Solubility Method
logp	0.958		Crippen Method
mccvol	88.750	ml/mol	McGowan Method
pc	3290.00 ± 20.00	kPa	NIST Webbook
rinpol	662.00		NIST Webbook
rinpol	611.00		NIST Webbook
rinpol	643.00		NIST Webbook
rinpol	650.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	645.00		NIST Webbook
rinpol	652.00		NIST Webbook
rinpol	648.00		NIST Webbook
rinpol	595.00		NIST Webbook
rinpol	643.00		NIST Webbook
rinpol	645.00		NIST Webbook
rinpol	650.00		NIST Webbook
rinpol	650.00		NIST Webbook
rinpol	648.00		NIST Webbook
rinpol	638.00		NIST Webbook
rinpol	643.00		NIST Webbook
rinpol	650.00		NIST Webbook
rinpol	648.00		NIST Webbook
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rinpol	648.00		NIST Webbook
rinpol	655.00		NIST Webbook
rinpol	648.00		NIST Webbook
rinpol	639.00		NIST Webbook
rinpol	639.00		NIST Webbook
rinpol	644.00		NIST Webbook
rinpol	657.10		NIST Webbook
rinpol	657.00		NIST Webbook
rinpol	643.00		NIST Webbook

rinpol	596.00		NIST Webbook
rinpol	610.00		NIST Webbook
rinpol	596.00		NIST Webbook
rinpol	643.00		NIST Webbook
rinpol	596.00		NIST Webbook
rinpol	646.80		NIST Webbook
rinpol	646.00		NIST Webbook
rinpol	625.00		NIST Webbook
rinpol	640.00		NIST Webbook
ripol	890.00		NIST Webbook
ripol	896.00		NIST Webbook
ripol	866.00		NIST Webbook
ripol	883.00		NIST Webbook
ripol	882.00		NIST Webbook
ripol	901.00		NIST Webbook
ripol	911.00		NIST Webbook
ripol	882.00		NIST Webbook
ripol	912.00		NIST Webbook
ripol	899.00		NIST Webbook
ripol	938.00		NIST Webbook
ripol	913.00		NIST Webbook
ripol	909.40		NIST Webbook
ripol	851.00		NIST Webbook
ripol	878.00		NIST Webbook
ripol	878.00		NIST Webbook
ripol	866.00		NIST Webbook
ripol	904.00		NIST Webbook
ripol	915.00		NIST Webbook
ripol	915.00		NIST Webbook
ripol	883.00		NIST Webbook
tb	361.45	K	Physical properties and phase equilibria of the system isopropyl acetate + isopropanol + 1-octyl-3-methyl-imidazolium bis(trifluoromethylsulfonyl)imide
tb	361.65	K	Isobaric vapor-liquid equilibrium data for the binary system methyl acetate + isopropyl acetate and the quaternary system methyl acetate + methanol + isopropanol + isopropyl acetate at 101.3 kPa
tb	361.79	K	Study of Vapor-Liquid Equilibria for Acetic Acid + n-Propyl Acetate + Isopropyl Acetate Systems

tb	361.79	K	Investigation on Isobaric Vapor-Liquid Equilibria of the Isopropyl Acetate + Water + Ethanol System
tb	361.45	K	Vapor Liquid Equilibria for Ternary Mixtures of Isopropyl Alcohol, Isopropyl Acetate, and DMSO at 101.3 kPa
tb	361.80	K	Experimental studies and thermodynamic analysis of isobaric vapor-liquid-liquid equilibria of 2-propanol + water system using n-propyl acetate and isopropyl acetate as entrainers
tc	532.00 ± 0.60	K	NIST Webbook
tc	531.00 ± 0.05	K	NIST Webbook
tf	203.85	K	NIST Webbook
tf	241.85 ± 0.50	K	NIST Webbook
tf	346.60 ± 0.50	K	NIST Webbook
tf	199.95	K	Aqueous Solubility Prediction Method
vc	0.334	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	158.99 ± 0.24	J/mol×K	376.91	NIST Webbook
cpg	154.31 ± 0.23	J/mol×K	361.35	NIST Webbook
cpg	163.59 ± 0.25	J/mol×K	392.36	NIST Webbook
cpg	168.95 ± 0.25	J/mol×K	411.00	NIST Webbook
cpl	196.60	J/mol×K	298.15	NIST Webbook
dvisc	0.0002653	Pa×s	389.65	Joback Method
dvisc	0.0043372	Pa×s	203.27	Joback Method
dvisc	0.0004730	Pa×s	327.52	Joback Method
dvisc	0.0019995	Pa×s	234.33	Joback Method
dvisc	0.0003455	Pa×s	358.59	Joback Method
dvisc	0.0011050	Pa×s	265.40	Joback Method
dvisc	0.0006915	Pa×s	296.46	Joback Method
hvapt	38.80	kJ/mol	298.50	NIST Webbook
hvapt	36.30	kJ/mol	318.00	NIST Webbook
hvapt	35.60	kJ/mol	323.00	NIST Webbook

pvap	36.19	kPa	332.14	Investigation on Isobaric Vapor-Liquid Equilibria of the Isopropyl Acetate + Water + Ethanol System
pvap	19.00	kPa	316.52	Investigation on Isobaric Vapor-Liquid Equilibria of the Isopropyl Acetate + Water + Ethanol System
pvap	20.00	kPa	317.77	Investigation on Isobaric Vapor-Liquid Equilibria of the Isopropyl Acetate + Water + Ethanol System
pvap	22.45	kPa	320.42	Investigation on Isobaric Vapor-Liquid Equilibria of the Isopropyl Acetate + Water + Ethanol System
pvap	25.60	kPa	323.45	Investigation on Isobaric Vapor-Liquid Equilibria of the Isopropyl Acetate + Water + Ethanol System
pvap	28.24	kPa	325.91	Investigation on Isobaric Vapor-Liquid Equilibria of the Isopropyl Acetate + Water + Ethanol System
pvap	31.94	kPa	328.97	Investigation on Isobaric Vapor-Liquid Equilibria of the Isopropyl Acetate + Water + Ethanol System
pvap	15.79	kPa	312.53	Investigation on Isobaric Vapor-Liquid Equilibria of the Isopropyl Acetate + Water + Ethanol System
pvap	39.98	kPa	334.75	Investigation on Isobaric Vapor-Liquid Equilibria of the Isopropyl Acetate + Water + Ethanol System

pvap	44.85	kPa	337.73	Investigation on Isobaric Vapor-Liquid Equilibria of the Isopropyl Acetate + Water + Ethanol System
pvap	50.51	kPa	340.95	Investigation on Isobaric Vapor-Liquid Equilibria of the Isopropyl Acetate + Water + Ethanol System
pvap	56.66	kPa	344.18	Investigation on Isobaric Vapor-Liquid Equilibria of the Isopropyl Acetate + Water + Ethanol System
pvap	60.03	kPa	345.94	Investigation on Isobaric Vapor-Liquid Equilibria of the Isopropyl Acetate + Water + Ethanol System
pvap	65.32	kPa	348.17	Investigation on Isobaric Vapor-Liquid Equilibria of the Isopropyl Acetate + Water + Ethanol System
pvap	13.35	kPa	308.95	Investigation on Isobaric Vapor-Liquid Equilibria of the Isopropyl Acetate + Water + Ethanol System
pvap	75.52	kPa	352.47	Investigation on Isobaric Vapor-Liquid Equilibria of the Isopropyl Acetate + Water + Ethanol System
pvap	79.97	kPa	354.29	Investigation on Isobaric Vapor-Liquid Equilibria of the Isopropyl Acetate + Water + Ethanol System

pvap	85.89	kPa	356.48	Investigation on Isobaric Vapor-Liquid Equilibria of the Isopropyl Acetate + Water + Ethanol System
pvap	90.50	kPa	358.20	Investigation on Isobaric Vapor-Liquid Equilibria of the Isopropyl Acetate + Water + Ethanol System
pvap	95.13	kPa	359.77	Investigation on Isobaric Vapor-Liquid Equilibria of the Isopropyl Acetate + Water + Ethanol System
pvap	101.26	kPa	361.79	Investigation on Isobaric Vapor-Liquid Equilibria of the Isopropyl Acetate + Water + Ethanol System
pvap	70.47	kPa	350.35	Investigation on Isobaric Vapor-Liquid Equilibria of the Isopropyl Acetate + Water + Ethanol System
pvap	60.00	kPa	345.94	Investigation on Isobaric Vapor-Liquid Equilibria of the Isopropyl Acetate + Water + Ethanol System
pvap	80.00	kPa	354.29	Investigation on Isobaric Vapor-Liquid Equilibria of the Isopropyl Acetate + Water + Ethanol System
pvap	101.30	kPa	361.79	Investigation on Isobaric Vapor-Liquid Equilibria of the Isopropyl Acetate + Water + Ethanol System
pvap	20.00	kPa	317.77	Study of Vapor-Liquid Equilibria for Acetic Acid + n-Propyl Acetate + Isopropyl Acetate Systems

pvap	40.00	kPa	334.75	Study of Vapor-Liquid Equilibria for Acetic Acid + n-Propyl Acetate + Isopropyl Acetate Systems
pvap	60.00	kPa	345.94	Study of Vapor-Liquid Equilibria for Acetic Acid + n-Propyl Acetate + Isopropyl Acetate Systems
pvap	80.00	kPa	354.29	Study of Vapor-Liquid Equilibria for Acetic Acid + n-Propyl Acetate + Isopropyl Acetate Systems
pvap	101.30	kPa	361.79	Study of Vapor-Liquid Equilibria for Acetic Acid + n-Propyl Acetate + Isopropyl Acetate Systems
pvap	37.73	kPa	333.15	Vapor-Liquid Equilibria on Seven Binary Systems: Ethylene Oxide + 2-Methylpropane; Acetophenone + Phenol; cis-1,3-Dichloropropene + 1,2-Dichloropropane; 1,5-Hexadiene + Allyl Chloride; Isopropyl Acetate + Acetonitrile; Vinyl Chloride + Methyl Chloride; and 1,4-Butanediol + c-Butyrolactone

pvap	249.59	kPa	393.15	Vapor-Liquid Equilibria on Seven Binary Systems: Ethylene Oxide + 2-Methylpropane; Acetophenone + Phenol; cis-1,3-Dichloropropene + 1,2-Dichloropropane; 1,5-Hexadiene + Allyl Chloride; Isopropyl Acetate + Acetonitrile; Vinyl Chloride + Methyl Chloride; and 1,4-Butanediol + c-Butyrolactone
pvap	939.90	kPa	453.15	Vapor-Liquid Equilibria on Seven Binary Systems: Ethylene Oxide + 2-Methylpropane; Acetophenone + Phenol; cis-1,3-Dichloropropene + 1,2-Dichloropropane; 1,5-Hexadiene + Allyl Chloride; Isopropyl Acetate + Acetonitrile; Vinyl Chloride + Methyl Chloride; and 1,4-Butanediol + c-Butyrolactone
pvap	11.58	kPa	306.28	Investigation on Isobaric Vapor-Liquid Equilibria of the Isopropyl Acetate + Water + Ethanol System
pvap	10.57	kPa	304.07	Investigation on Isobaric Vapor-Liquid Equilibria of the Isopropyl Acetate + Water + Ethanol System
pvap	101.30	kPa	361.45	Vapor Liquid Equilibria for Ternary Mixtures of Isopropyl Alcohol, Isopropyl Acetate, and DMSO at 101.3 kPa

pvap	251.71	kPa	393.99	Vapor-Liquid Equilibrium of Binary Mixtures Containing Isopropyl Acetate and Alkanols at 101.32 kPa	
pvap	201.37	kPa	385.39	Vapor-Liquid Equilibrium of Binary Mixtures Containing Isopropyl Acetate and Alkanols at 101.32 kPa	
pvap	151.03	kPa	375.00	Vapor-Liquid Equilibrium of Binary Mixtures Containing Isopropyl Acetate and Alkanols at 101.32 kPa	
pvap	125.86	kPa	368.80	Vapor-Liquid Equilibrium of Binary Mixtures Containing Isopropyl Acetate and Alkanols at 101.32 kPa	
pvap	100.54	kPa	361.41	Vapor-Liquid Equilibrium of Binary Mixtures Containing Isopropyl Acetate and Alkanols at 101.32 kPa	
pvap	101.00	kPa	361.80	Experimental studies and thermodynamic analysis of isobaric vapor-liquid-liquid equilibria of 2-propanol + water system using n-propyl acetate and isopropyl acetate as entrainers	
pvap	176.20	kPa	380.40	Vapor-Liquid Equilibrium of Binary Mixtures Containing Isopropyl Acetate and Alkanols at 101.32 kPa	
pvap	40.00	kPa	334.75	Investigation on Isobaric Vapor-Liquid Equilibria of the Isopropyl Acetate + Water + Ethanol System	

pvap	226.54	kPa	389.89	Vapor-Liquid Equilibrium of Binary Mixtures Containing Isopropyl Acetate and Alkanols at 101.32 kPa
rfi	1.37710		293.15	Liquid Liquid Equilibrium for the Ternary System Isopropyl Acetate + Ethanol + Water at (293.15, 313.15, and 333.15) K
rfi	1.37010		303.15	Liquid-liquid equilibrium for ternary systems of ethyl acetate/isopropyl acetate + 2,2,3,3-tetrafluoro-1-propanol + water at 298.15, 318.15 K
rfi	1.37790		293.15	Liquid-liquid equilibria of water + solutes (acetic acid/ acetol/furfural/guaiacol/methanol/phenol/propanal) + solvents (isopropyl acetate/toluene) ternary systems for pyrolysis oil fractionation
rfi	1.37720		293.15	Isobaric Vapor-Liquid Equilibria for Water + Acetic Acid + (n-Pentyl Acetate or Isopropyl Acetate)
rfi	1.37739		298.15	Isobaric Vapor-Liquid Equilibrium Data for Binary Systems of Anisole with Methyl Acetate, Ethyl Acetate, n-Propyl Acetate, and Isopropyl Acetate at 93.9 kPa

rfi	1.37480		298.15	Vapor-Liquid Equilibrium Data for Binary Mixtures of Dimethyl Carbonate with Methyl Acetate, Ethyl Acetate, n-Propyl Acetate, Isopropyl Acetate, n-Butyl Acetate, and Isoamyl Acetate at 93.13 kPa
rfi	1.37480		298.15	Isobaric vapour liquid equilibria and physical properties for isopropyl acetate + isopropanol + 1-butyl-3-methyl-imidazolium bis(trifluoromethylsulfonyl)imide mixtures
rfi	1.37510		293.15	Vapor liquid equilibria of carbon dioxide with isopropyl acetate, diethyl carbonate and ethyl butyrate at elevated pressures
rhoI	867.60	kg/m3	298.15	Determination and Correlation of Liquid-Liquid Equilibria Data for Ternary System Isopropyl Acetate + Isopropanol + Water at Different Temperatures
srf	0.02	N/m	308.15	Excess Molar Volumes and Surface Tensions of 1,2,4-Trimethylbenzene and 1,3,5-Trimethylbenzene with Isopropyl Acetate and Isobutyl Acetate at (298.15, 308.15, and 313.15) K

srf	0.02	N/m	298.15	Excess Molar Volumes and Surface Tensions of 1,2,4-Trimethylbenzene and 1,3,5-Trimethylbenzene with Isopropyl Acetate and Isobutyl Acetate at (298.15, 308.15, and 313.15) K
srf	0.02	N/m	313.15	Excess Molar Volumes and Surface Tensions of 1,2,4-Trimethylbenzene and 1,3,5-Trimethylbenzene with Isopropyl Acetate and Isobutyl Acetate at (298.15, 308.15, and 313.15) K

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	4.79142e+01
Coeff. B	-5.71639e+03
Coeff. C	-4.70480e+00
Coeff. D	1.64122e-06
Temperature range (K), min.	199.75
Temperature range (K), max.	538.00

Datasets

Mass density, kg/m3

Temperature, K - Liquid

Pressure, kPa - Liquid

Mass density, kg/m3 - Liquid

<https://www.doi.org/10.1016/j.fluid.2017.09.010>
<http://link.springer.com/article/10.1007/BF02311772>
<https://www.doi.org/10.1021/acs.jced.6b00040>
<https://www.doi.org/10.1021/acs.jced.8b00844>
<https://www.doi.org/10.1016/j.fluid.2019.06.016>
<https://www.doi.org/10.1021/acs.jced.8b00776>
<https://www.doi.org/10.1016/j.fluid.2004.12.005>
<https://www.doi.org/10.1021/acs.jced.8b00063>
<https://www.doi.org/10.1021/acs.jced.6b00415>
<https://www.doi.org/10.1021/acs.jced.6b00428>
<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>
<https://www.doi.org/10.1016/j.jct.2016.12.006>
<https://www.doi.org/10.1021/je400245u>
<https://www.doi.org/10.1021/acs.jced.9b00152>
<https://www.doi.org/10.1021/je800120p>
<https://www.doi.org/10.1021/je050317k>
<https://www.doi.org/10.1021/je100125x>
<https://www.doi.org/10.1016/j.fluid.2009.03.006>
<https://www.doi.org/10.1016/j.fluid.2009.09.015>
<https://www.doi.org/10.1021/acs.jced.5b00746>
<https://www.doi.org/10.1021/acs.jced.7b00194>
https://en.wikipedia.org/wiki/Joback_method
<https://www.doi.org/10.1021/acs.jced.9b00595>
<https://www.doi.org/10.1016/j.fluid.2010.10.003>
<https://www.doi.org/10.1021/je049711t>
<https://www.doi.org/10.1016/j.fluid.2005.05.018>
<https://www.doi.org/10.1021/acs.jced.9b00658>
<https://www.doi.org/10.1016/j.fluid.2015.12.050>
<http://webbook.nist.gov/cgi/cbook.cgi?ID=C108214&Units=SI>
<https://www.doi.org/10.1021/je800046k>
<https://www.doi.org/10.1021/acs.jced.7b00704>
<https://www.doi.org/10.1016/j.fluid.2009.03.008>
<https://www.doi.org/10.1021/je060321b>
http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
<https://www.doi.org/10.1016/j.fluid.2013.01.024>

Liquid-liquid equilibria of water + solutes (acetic acid/
acetone/tetrahydrofuran/methanol/propanal)
Measures Coexisting Liquid Phases
Chemical Vapor Pressure Data:
KDB Vapor Pressure Data:

Measurement and thermodynamic modelling of ternary liquid-liquid equilibrium for ethanol-Vapor-Liquid Equilibria of Ethyl Formate-Acetate-Water Binary Systems
When different Solvents
4-hydroxy-2,5-dimethyl-3(2H)-furanone
In Different Solvents
Binary Mixtures of Diethyl Carbonate
Measurements and Correlation of
Acetate or Isoamyl Acetate at 101.3 kPa
acid in pure solvents:

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
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
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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