

Isobutyl acetate

Other names:	2-METHYL-1-PROPYL ACETATE
	2-METHYLPROPYL ESTER ACETIC ACID
	2-Methyl-1-propanol, acetate
	2-Methylpropyl acetate
	2-Methylpropyl ethanoate
	Acetate d'isobutyle
	Acetic acid, 2-methylpropyl ester
	Acetic acid, isobutyl ester
	ISOBUTYL ETHANOATE
	Isobutyl acetate fcc
	Isobutylester kyseliny octove
	NSC 8035
	UN 1213
	ethanoic acid, isobutyl ester
	i-Butyl acetate
	«beta»-Methylpropyl ethanoate
	Â«betaÂ»-Methylpropyl ethanoate
Inchi:	InChI=1S/C6H12O2/c1-5(2)4-8-6(3)7/h5H,4H2,1-3H3
InchiKey:	GJRQTCIYDGXPES-UHFFFAOYSA-N
Formula:	C6H12O2
SMILES:	CC(=O)OCC(C)C
Mol. weight [g/mol]:	116.16
CAS:	110-19-0

Physical Properties

Property code	Value	Unit	Source
af	0.4550		KDB
aigt	695.93	K	KDB
chl	-3534.00	kJ/mol	NIST Webbook
dm	1.90	debye	KDB
fll	2.40	% in Air	KDB
flu	10.50	% in Air	KDB
fpc	302.59	K	KDB
fpo	289.82	K	KDB
gf	-236.72	kJ/mol	Joback Method
hf	-495.50	kJ/mol	KDB
hfus	10.56	kJ/mol	Joback Method

hvap	35.90 ± 0.04	kJ/mol	NIST Webbook
ie	9.97	eV	NIST Webbook
log10ws	-1.21		Estimated Solubility Method
log10ws	-1.21		Aqueous Solubility Prediction Method
logp	1.205		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=1)		KDB
pc	3180.00 ± 60.79	kPa	NIST Webbook
pc	3010.00 ± 20.00	kPa	NIST Webbook
pc	3160.00	kPa	KDB
rhoc	281.10 ± 8.13	kg/m3	NIST Webbook
rinpol	752.10		NIST Webbook
rinpol	748.00		NIST Webbook
rinpol	755.00		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	754.00		NIST Webbook
rinpol	759.00		NIST Webbook
rinpol	762.00		NIST Webbook
rinpol	749.00		NIST Webbook
rinpol	762.00		NIST Webbook
rinpol	759.00		NIST Webbook
rinpol	758.00		NIST Webbook
rinpol	749.00		NIST Webbook
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rinpol	758.00		NIST Webbook
rinpol	753.00		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	767.00		NIST Webbook
rinpol	753.00		NIST Webbook
rinpol	758.00		NIST Webbook
rinpol	768.00		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	768.00		NIST Webbook
rinpol	781.00		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	771.00		NIST Webbook
rinpol	782.00		NIST Webbook
rinpol	780.00		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	758.00		NIST Webbook

rinpol	746.00	NIST Webbook
rinpol	764.00	NIST Webbook
rinpol	758.00	NIST Webbook
rinpol	754.00	NIST Webbook
rinpol	744.00	NIST Webbook
rinpol	743.00	NIST Webbook
rinpol	745.00	NIST Webbook
rinpol	744.00	NIST Webbook
rinpol	758.00	NIST Webbook
rinpol	770.00	NIST Webbook
rinpol	760.00	NIST Webbook
rinpol	760.00	NIST Webbook
rinpol	764.00	NIST Webbook
rinpol	757.00	NIST Webbook
rinpol	779.50	NIST Webbook
rinpol	767.00	NIST Webbook
rinpol	770.00	NIST Webbook
rinpol	764.00	NIST Webbook
rinpol	749.00	NIST Webbook
rinpol	734.00	NIST Webbook
rinpol	766.00	NIST Webbook
rinpol	757.00	NIST Webbook
rinpol	771.00	NIST Webbook
rinpol	768.00	NIST Webbook
rinpol	776.00	NIST Webbook
rinpol	763.00	NIST Webbook
rinpol	786.00	NIST Webbook
rinpol	780.00	NIST Webbook
rinpol	782.00	NIST Webbook
rinpol	749.00	NIST Webbook
rinpol	749.00	NIST Webbook
rinpol	750.00	NIST Webbook
rinpol	748.00	NIST Webbook
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rinpol	770.00	NIST Webbook
rinpol	753.00	NIST Webbook
rinpol	780.00	NIST Webbook
rinpol	750.00	NIST Webbook
rinpol	758.00	NIST Webbook
rinpol	746.00	NIST Webbook
rinpol	747.00	NIST Webbook
rinpol	771.00	NIST Webbook
rinpol	730.00	NIST Webbook
rinpol	781.00	NIST Webbook

rinpol	768.00	NIST Webbook
rinpol	754.00	NIST Webbook
rinpol	754.00	NIST Webbook
rinpol	754.45	NIST Webbook
rinpol	748.70	NIST Webbook
rinpol	749.80	NIST Webbook
rinpol	753.00	NIST Webbook
rinpol	759.00	NIST Webbook
rinpol	750.00	NIST Webbook
rinpol	749.70	NIST Webbook
rinpol	757.70	NIST Webbook
rinpol	758.98	NIST Webbook
rinpol	757.00	NIST Webbook
rinpol	755.00	NIST Webbook
rinpol	757.20	NIST Webbook
rinpol	750.00	NIST Webbook
rinpol	768.00	NIST Webbook
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rinpol	748.00	NIST Webbook
rinpol	760.00	NIST Webbook
rinpol	746.00	NIST Webbook
rinpol	750.00	NIST Webbook
rinpol	783.00	NIST Webbook
rinpol	788.00	NIST Webbook
rinpol	753.00	NIST Webbook
rinpol	767.20	NIST Webbook
rinpol	741.00	NIST Webbook
rinpol	741.00	NIST Webbook
rinpol	781.00	NIST Webbook
rinpol	779.00	NIST Webbook
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rinpol	755.00	NIST Webbook
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rinpol	770.00	NIST Webbook
rinpol	745.30	NIST Webbook
rinpol	748.40	NIST Webbook
rinpol	764.00	NIST Webbook

ripol	758.00	NIST Webbook
ripol	976.00	NIST Webbook
ripol	1025.00	NIST Webbook
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ripol	1033.00	NIST Webbook
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ripol	1020.00	NIST Webbook
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ripol	1020.00	NIST Webbook
ripol	1020.00	NIST Webbook
ripol	1017.00	NIST Webbook
ripol	985.00	NIST Webbook
ripol	1024.00	NIST Webbook
ripol	1005.00	NIST Webbook
ripol	1012.00	NIST Webbook
ripol	1012.00	NIST Webbook
ripol	1020.00	NIST Webbook
ripol	1019.00	NIST Webbook
ripol	1047.00	NIST Webbook
ripol	1014.00	NIST Webbook
ripol	1014.00	NIST Webbook
ripol	1011.00	NIST Webbook
ripol	1010.00	NIST Webbook
ripol	1017.00	NIST Webbook
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ripol	1005.00	NIST Webbook
ripol	1005.00	NIST Webbook
ripol	1007.00	NIST Webbook
ripol	1014.00	NIST Webbook
ripol	1005.00	NIST Webbook
ripol	1000.00	NIST Webbook

ripol	1005.00		NIST Webbook
ripol	992.00		NIST Webbook
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ripol	1000.00		NIST Webbook
ripol	1009.00		NIST Webbook
ripol	1000.00		NIST Webbook
ripol	1008.00		NIST Webbook
ripol	1032.00		NIST Webbook
ripol	1004.00		NIST Webbook
ripol	1015.00		NIST Webbook
ripol	985.00		NIST Webbook
ripol	1035.00		NIST Webbook
ripol	1009.00		NIST Webbook
ripol	1009.00		NIST Webbook
ripol	1012.00		NIST Webbook
ripol	1010.00		NIST Webbook
ripol	1034.00		NIST Webbook
ripol	1016.00		NIST Webbook
ripol	1018.00		NIST Webbook
ripol	1012.00		NIST Webbook
ripol	1009.00		NIST Webbook
ripol	1009.00		NIST Webbook
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ripol	1014.00		NIST Webbook
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ripol	989.00		NIST Webbook
ripol	1027.00		NIST Webbook
ripol	1007.00		NIST Webbook
ripol	1002.00		NIST Webbook
ripol	1022.00		NIST Webbook
ripol	1029.00		NIST Webbook
ripol	1031.00		NIST Webbook
ripol	1000.00		NIST Webbook
ripol	1017.00		NIST Webbook
ripol	1002.00		NIST Webbook
tb	389.44	K	Isobaric VLE at 0.6 MPa for binary systems isobutyl acetate + ethanol, + 1-propanol or + 2-propanol

tb	389.55	K	Vapour-liquid equilibrium measurements and extractive distillation process design for separation of azeotropic mixture (dimethyl carbonate + ethanol)
tb	389.55	K	Isobaric Vapor-Liquid Equilibrium Measurements for Separation of Azeotrope (Methanol + Methyl Acetate)
tb	389.75	K	Measurement and Correlation of Isobaric Vapor-Liquid Equilibrium for Binary Systems of Allyl Alcohol with Isobutyl Acetate, Butyl Acetate, and Butyl Propionate at 101.3 kPa
tb	389.90	K	Isobaric Vapor Liquid Equilibrium for the Binary and Ternary System with Isobutyl Alcohol, Isobutyl Acetate and Dimethyl Sulfoxide at 101.3 kPa
tb	389.70	K	KDB
tc	561.50 ± 2.00	K	NIST Webbook
tc	569.00 ± 5.00	K	NIST Webbook
tc	561.00	K	KDB
tc	560.80 ± 0.60	K	NIST Webbook
tf	174.25	K	Aqueous Solubility Prediction Method
tf	174.30	K	KDB
tf	176.05	K	NIST Webbook
tf	176.10 ± 0.60	K	NIST Webbook
tf	240.15 ± 0.50	K	NIST Webbook
vc	0.414	m3/kmol	KDB
zc	0.2804710		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.90	J/mol×K	412.53	Joback Method
cpg	210.06	J/mol×K	442.81	Joback Method
cpg	219.89	J/mol×K	473.09	Joback Method
cpg	229.39	J/mol×K	503.38	Joback Method
cpg	238.55	J/mol×K	533.66	Joback Method
cpg	247.38	J/mol×K	563.94	Joback Method

cpg	255.87	J/mol×K	594.22	Joback Method
cpl	240.20	J/mol×K	290.00	NIST Webbook
dvisc	0.0020807	Pa×s	247.54	Joback Method
dvisc	0.0011317	Pa×s	280.54	Joback Method
dvisc	0.0006998	Pa×s	313.53	Joback Method
dvisc	0.0004742	Pa×s	346.53	Joback Method
dvisc	0.0003438	Pa×s	379.53	Joback Method
dvisc	0.0002624	Pa×s	412.53	Joback Method
dvisc	0.0046134	Pa×s	214.54	Joback Method
hvapt	39.80	kJ/mol	321.50	NIST Webbook
hvapt	39.20	kJ/mol	359.00	NIST Webbook
hvapt	39.90	kJ/mol	349.50	NIST Webbook
pvap	101.30	kPa	389.55	Vapour-liquid equilibrium measurements and extractive distillation process design for separation of azeotropic mixture (dimethyl carbonate + ethanol)
rfi	1.38760		298.15	Vapor liquid equilibria in the ternary system isobutyl alcohol + isobutyl acetate + butyl propionate and the binary systems isobutyl alcohol + butyl propionate, isobutyl acetate + butyl propionate at 101.3 kPa
rfi	1.39020		293.15	Measurement and Correlation of Phase Equilibria for Isobutyl Acetate + {Ethanol or Methanol} + Water at 303.15 and 323.15 K
rfi	1.38780		298.20	Tie-line data for the aqueous solutions of phenol with organic solvents at T = 298.2 K

rfi	1.38760	298.15	Study of liquid liquid equilibrium of the systems isobutyl acetate + acetic acid +water and isobutyl alcohol + acetic acid +water at different temperatures
rfi	1.38760	298.15	Liquid liquid equilibria of the systems isobutyl acetate + isobutyl alcohol +water and isobutyl acetate + isobutyl alcohol + glycerol at different temperatures
rfi	1.38760	298.15	Isobaric vapor-liquid equilibria for the binary systems isobutyl alcohol + isobutyl acetate and tert-butyl alcohol + tert-butyl acetate at 20 and 101.3 kPa
rfi	1.38760	298.15	Phase equilibria in the systems isobutyl alcohol +N,N-dimethylformamide, isobutyl acetate +N,N-dimethylformamide and isobutyl alcohol + isobutyl acetate +N,N-dimethylformamide at 101.3 kPa
rfi	1.39050	293.15	Isobaric Vapor Liquid Equilibrium for Binary Systems of Thioglycolic Acid with Water, Butyl Acetate, Butyl Formate, and Isobutyl Acetate at 101.3 kPa

rfi	1.38760		298.15	Phase equilibria in the ternary system isobutyl alcohol + isobutyl acetate + 1-hexanol and the binary systems isobutyl alcohol + 1-hexanol, isobutyl acetate + 1-hexanol at 101.3 kPa
rhoI	875.00	kg/m3	293.00	KDB
rhoI	871.30	kg/m3	293.20	Liquid-liquid equilibrium data for ternary systems of water + acetic acid + acetate esters at 293.2 K and 303.2 K and ~ 95 kPa
rhoI	849.39	kg/m3	313.20	Liquid-liquid equilibrium data for ternary systems of water + acetic acid + acetate esters at 293.2 K and 303.2 K and ~ 95 kPa
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
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
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Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbp	361.00	K	39.99	Vapor Liquid Equilibrium for Binary Mixtures of Acetates in the Direct Esterification of Fusel Oil
tbp	367.41	K	49.98	Vapor Liquid Equilibrium for Binary Mixtures of Acetates in the Direct Esterification of Fusel Oil
tbp	372.89	K	59.99	Vapor Liquid Equilibrium for Binary Mixtures of Acetates in the Direct Esterification of Fusel Oil
tbp	377.39	K	70.00	Vapor Liquid Equilibrium for Binary Mixtures of Acetates in the Direct Esterification of Fusel Oil
tbp	381.58	K	80.00	Vapor Liquid Equilibrium for Binary Mixtures of Acetates in the Direct Esterification of Fusel Oil

tbp	385.54	K	90.00	Vapor Liquid Equilibrium for Binary Mixtures of Acetates in the Direct Esterification of Fusel Oil
tbp	389.37	K	100.00	Vapor Liquid Equilibrium for Binary Mixtures of Acetates in the Direct Esterification of Fusel Oil
tbp	392.35	K	110.00	Vapor Liquid Equilibrium for Binary Mixtures of Acetates in the Direct Esterification of Fusel Oil
tbp	395.26	K	120.00	Vapor Liquid Equilibrium for Binary Mixtures of Acetates in the Direct Esterification of Fusel Oil
tbp	398.16	K	130.00	Vapor Liquid Equilibrium for Binary Mixtures of Acetates in the Direct Esterification of Fusel Oil
tbp	400.84	K	140.00	Vapor Liquid Equilibrium for Binary Mixtures of Acetates in the Direct Esterification of Fusel Oil
tbp	403.64	K	150.00	Vapor Liquid Equilibrium for Binary Mixtures of Acetates in the Direct Esterification of Fusel Oil

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$

Coeff. A	1.50519e+01
Coeff. B	-3.64415e+03
Coeff. C	-4.07290e+01
Temperature range (K), min.	287.55
Temperature range (K), max.	414.85

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	9.01223e+01
Coeff. B	-7.87047e+03
Coeff. C	-1.11424e+01
Coeff. D	7.93342e-06
Temperature range (K), min.	174.30
Temperature range (K), max.	561.00

Sources

Solubility of Lovastatin in Ethyl Acetate, Propyl Acetate, Isopropyl Acetate, n-Propyl Acetate, sec-Butyl Acetate, Isobutyl Acetate, tert-Butyl Acetate, and 2-Butanone, between 285 K and 325 K (for ethyl acetate or iso-butyl acetate):

<https://www.doi.org/10.1021/je800120p>

Liquid liquid equilibria of the systems isobutyl acetate + isobutyl alcohol + water and isobutyl acetate + isobutyl alcohol + 2-methyl propyl acetate in different proportions of solvents in the presence of menthane in Isobutyl Acetate, n-Butyric Acid, Ethyl Acetate, and 2-Butanone. Solubility of Benzene, Acetic Acid and Aspirin in Different Solvents Using a Laser Raman Scattering Method. Vapor pressure measurements and extractive distillation of isobutyl acetate + isobutyl alcohol + 2-methyl propyl acetate + water. Solubility of isobutyl acetate + isobutyl alcohol + 2-methyl propyl acetate + water.

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C110190&Units=SI>

<https://www.doi.org/10.1016/j.fluid.2011.03.006>

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

<https://www.doi.org/10.1016/j.fluid.2008.01.010>

<https://www.doi.org/10.1016/j.fluid.2009.03.006>

<https://www.doi.org/10.1021/je800428r>

<https://www.doi.org/10.1021/acs.jced.5b00746>

<https://www.doi.org/10.1016/j.jct.2019.01.027>

<https://www.doi.org/10.1021/je2003226>

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

Excess Molar Volumes and Surface Tensions of 1,2,4-Trimethylbenzene and Determination of Binary Vapor Liquid Equilibria of CO₂-Based Acetate Mixtures. Solubility of Benzene in Isobutyl Acetate + Isobutyl Alcohol + 2-Methyl Propyl Acetate + Water at 303.15 and 323.15 K. Solubilities of Benzene Carboxylic Acids in Isobutyl Acetate from (299.73 to 323.15 K) in the ternary system isobutyl alcohol + isobutyl acetate + isobutyl alcohol + 2-methyl propyl acetate. Systems isobutyl acetate + isobutyl alcohol + 2-methyl propyl acetate + water. Liquid liquid equilibria for the Ternary Systems Acetic Acid + Water + Butyl Acetate and Acetic Acid + Water + 2-Methyl Propyl Acetate at 304.15 K, 302.15 K, and 306.15 K. Solubility of lansoprazole in different solvents:

<https://www.doi.org/10.1021/je800046k>

<https://www.doi.org/10.1021/je501023n>

<https://www.doi.org/10.1021/acs.jced.6b00949>

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

<https://www.doi.org/10.1021/je101319f>

<https://www.doi.org/10.1016/j.fluid.2005.06.019>

<https://www.doi.org/10.1016/j.fluid.2012.06.013>

<https://www.doi.org/10.1021/acs.jced.8b01045>

<https://www.doi.org/10.1021/je6005746>

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

<https://www.doi.org/10.1016/j.fluid.2012.06.011>

Separation of Protocatechuic Acid Using Di-(2-ethylhexyl)phosphoric Acid Vapor-Liquid Equilibrium for Binary Mixtures of Acetates in the Direct Rectification and Generation of Isobaric Vapor-Liquid Equilibrium for Solution Thermodynamic of Alcohol with Simple Aromatic and Aliphatic Acids Isobaric Vapor-Liquid Equilibrium for the Binary and Ternary System with Vapor-Liquid Equilibrium in the Ternary System Isobaric Liquid-Liquid Phase Behavior of Binary and Ternary Systems for the Isopropyl Acetate and Isopropyl Propionate in Supercritical butyl propionate, isobutyl acetate + butyl propionate at 101.3 kPa:

<https://www.doi.org/10.1016/j.fluid.2013.12.026>

Legend

af:	Acentric Factor
ai_{gt}:	Autoignition Temperature
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
fl_l:	Lower Flammability Limit
fl_u:	Upper Flammability Limit
fpc:	Flash Point (Closed Cup Method)
fpo:	Flash Point (Open Cup Method)
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
rhoc:	Critical density
rhof:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tbp:	Boiling point at given pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility

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