sec-Butyl acetate

Other names:	1-Methylpropyl acetate
	1-Methylpropyl ethanoate
	2-Butanol acetate
	2-Butyl acetate
	Acetate de butyle secondaire
	Acetic acid, 1-methylpropyl ester
	Acetic acid, 2-butoxy ester
	Acetic acid, sec-butyl ester
	CH3COOCH(CH3)C2H5
	NSC 8034
	dl-sec-Butyl acetate
	sec-Butyl alcohol acetate
	sec-Butyl ethanoate
Inchi:	InChI=1S/C6H12O2/c1-4-5(2)8-6(3)7/h5H,4H2,1-3H3
InchiKey:	DCKVNWZUADLDEH-UHFFFAOYSA-N
Formula:	C6H12O2
SMILES:	CCC(C)OC(C)=O
Mol. weight [g/mol]:	116.16
CAS:	105-46-4

Physical Properties

Property code	Value	Unit	Source
gf	-236.72	kJ/mol	Joback Method
hf	-417.25	kJ/mol	Joback Method
hfus	10.56	kJ/mol	Joback Method
hvap	37.72	kJ/mol	Joback Method
ie	9.91 ± 0.03	eV	NIST Webbook
ie	9.97 ± 0.05	eV	NIST Webbook
ie	9.90	eV	NIST Webbook
ie	9.90	eV	NIST Webbook
log10ws	-1.31		Crippen Method
logp	1.348		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
rinpol	758.00		NIST Webbook
rinpol	746.00		NIST Webbook
rinpol	744.00		NIST Webbook

rinpol	746.00		NIST Webbook
rinpol	749.00		NIST Webbook
rinpol	746.00		NIST Webbook
rinpol	740.00		NIST Webbook
rinpol	738.10		NIST Webbook
rinpol	746.00		NIST Webbook
rinpol	737.00		NIST Webbook
rinpol	749.00		NIST Webbook
rinpol	745.00		NIST Webbook
rinpol	738.00		NIST Webbook
ripol	988.00		NIST Webbook
ripol	974.00		NIST Webbook
ripol	985.00		NIST Webbook
ripol	982.00		NIST Webbook
ripol	993.00		NIST Webbook
ripol	985.00		NIST Webbook
ripol	990.00		NIST Webbook
ripol	974.00		NIST Webbook
ripol	974.00		NIST Webbook
tb	385.00	K	NIST Webbook
tb	385.20	K	Investigation on Isobaric Vapor Liquid Equilibrium for Water + Acetic Acid + sec-Butyl Acetate
tb	385.40	K	NIST Webbook
tb	385.25	K	Experimental Measurements of Vapor Liquid Equilibrium Data for the Binary Systems of Methanol + 2-Butyl Acetate, 2-Butyl Alcohol + 2-Butyl Acetate, and Methyl Acetate + 2-Butyl Acetate at 101.33 kPa
tb	384.00 ± 3.00	K	NIST Webbook
tb	383.20 ± 2.00	K	NIST Webbook
tb	385.00 ± 2.00	K	NIST Webbook
tb	389.65 ± 1.00	K	NIST Webbook
tb	385.35 ± 1.00	K	NIST Webbook
tb	385.15	K	Isobaric Vapor-Liquid Equilibrium for the Binary Systems of 1,2-Dichloroethane + sec-Butyl Acetate, n-Propyl Acetate, and tert-Butyl Acetate at 101.3 kPa

tb	385.15	K	Isobaric Vapor-Liquid Equilibrium for Two Binary Systems of n-Heptane + sec-Butyl Acetate and Methylcyclohexane + sec-Butyl Acetate under Atmosphere
tb	385.12	K	Isobaric Vapor Liquid Equilibrium for the Binary Systems of sec-Butyl Acetate + n-Butyl Alcohol, Isobutyl Alcohol, or tert-Butyl Alcohol at 101.3 kPa
tb	385.33	K	Experimental isobaric vapour-liquid equilibrium data for the binary system (N, N-dimethyl acetamide + dimethyl sulfoxide) and the quaternary system (sec-butyl acetate + sec-butyl alcohol + N, N-dimethyl acetamide + dimethyl sulfoxide) at 101.3 kPa
tc	594.22	K	Joback Method
tf	214.54	K	Joback Method
vc	0.390	m3/kmol	Joback Method

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
dvisc	0.0002624	Pa×s	412.53	Joback Method
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	0.0046134	Pa×s	214.54	Joback Method
dvisc	0.0003438	Pa×s	379.53	Joback Method
dvisc	0.0004742	Pa×s	346.53	Joback Method

pvap	101.30	kPa	385.15	Isobaric Vapor-Liquid Equilibrium for Two Binary Systems of n-Heptane + sec-Butyl Acetate and Methylcyclohexane + sec-Butyl Acetate under Atmosphere
pvap	101.30	kPa	385.15	Isobaric Vapor-Liquid Equilibrium for the Binary Systems of 1,2-Dichloroethane + sec-Butyl Acetate, n-Propyl Acetate, and tert-Butyl Acetate at 101.3 kPa
pvap	101.33	kPa	385.25	Experimental Measurements of Vapor Liquid Equilibrium Data for the Binary Systems of Methanol + 2-Butyl Acetate, 2-Butyl Alcohol + 2-Butyl Acetate, and Methyl Acetate + 2-Butyl Acetate at 101.33 kPa
rfi	1.38700		298.15	Liquid-Liquid Equilibria for the System 1-Methyl Propyl Ethanoate (1) + Acetic Acid (2) + Water (3) at (283.15 and 323.15) K
rhol	866.40	kg/m3	298.15	Isobaric vapor-liquid equilibrium of the binary system sec-butyl acetate + para-xylene and the quaternary system methyl acetate + para-xylene + sec-butyl acetate + acetic acid at 101.3 kPa

rhol	871.00	kg/m3	293.15	Liquid - liquid equilibrium for the quaternary reaction system water p sec-butyl alcohol p sec-butyl acetate p acetic acid
rhol	863.80	kg/m3	298.15	Isobaric Vapor Liquid Equilibrium for the Binary Systems of sec-Butyl Acetate + Methyl Ethyl Ketone, 2-Methoxyethanol, or 1,2-Dimethoxyethane at 101.3 kPa
rhol	867.00	kg/m3	298.15	Isobaric Vapor-Liquid Equilibrium for the Binary Systems of Sec-butyl Acetate and Ethanol, 1-Propanol, or 2-Propanol at 101.3 kPa

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.94870e+01
Coeff. B	-5.11855e+03
Coeff. C	-1.39214e-01
Coeff. D	-4.69511e-06
Temperature range (K), min.	313.15
Temperature range (K), max.	523.15

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
298.15	100.00	865.5

Reference *https://www.doi.org/10.1021/acs.jced.9b00430*

Sources

Isobaric vapor-liquid equilibrium of the binary system sec-butyl acetate + 1-butanol and the quaternary system water + sec-butyl acetate + 1-butanol at 101.3 kPa:	https://www.doi.org/10.1016/j.fluid.2015.05.032
Isobaric Vapor-Liquid Equilibria for the Binary Systems of sec-Butyl Acetate + Methanol, + 2-Butanol, or 2-Propanol at 101.3 kPa:	https://www.doi.org/10.1021/acs.jced.6b00471
Isobaric Vapor-Liquid Equilibrium for the Binary Systems of sec-Butyl Acetate + Acetic Acid at 101.3 kPa:	https://www.doi.org/10.1021/acs.jced.7b00445
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1081
Liquid-Liquid Equilibria for the System 1-Methyl Propyl Ethanoate (1) + Acetic Acid (2) + Water (3) at (288.15 and 323.15) K:	https://www.doi.org/10.1021/je900332x
Liquid-liquid equilibria for the quaternary reaction system water p	https://www.doi.org/10.1016/j.fluid.2016.10.027
Isobaric Vapor-Liquid Equilibrium for Ternary System of sec-Butyl alcohol + sec-Butyl Acetate + N,N-dimethyl acetamide at 101.3 kPa:	https://www.doi.org/10.1016/j.fluid.2015.03.013
Isobaric Vapor-Liquid Equilibria of Binary Mixtures of Diethyl Carbonate with Isopropyl Acetate, sec-Butyl Acetate, or Isoamyl Acetate at 101.3 kPa:	https://www.doi.org/10.1021/acs.jced.9b00430
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Investigation on Isobaric Vapor Liquid Equilibrium for Water + Acetic Acid + sec-Butyl Acetate:	https://www.doi.org/10.1021/je500160t
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C105464&Units=SI
Experimental Measurements of Vapor Liquid Equilibrium Data for the Binary Systems of Methanol + 2-Butyl Acetate, 2-Butyl Alcohol + 2-Butyl Acetate, and Methyl Acetate + 2-Butyl Acetate at Isobaric Conditions of Normal Atmosphere:	https://www.doi.org/10.1021/je400226q
Isobaric Vapor-Liquid Equilibrium for Two Binary Systems of n-Heptane + sec-Butyl Acetate and n-Heptane + tert-Butyl Acetate at 101.3 kPa:	https://www.doi.org/10.1021/acs.jced.7b00999
Experimental isobaric vapor-liquid equilibrium for the ternary system of sec-butyl acetate + 2-butanol + 2-propanol at 101.3 kPa:	https://www.doi.org/10.1016/j.fluid.2015.07.029
Solubility and limiting activity coefficients of simvastatin in different organic solvents:	https://www.doi.org/10.1016/j.fluid.2009.03.006
Liquid–liquid equilibrium of the ternary system water + acetic acid + sec-butyl acetate:	https://www.doi.org/10.1016/j.fluid.2010.01.005
Solubility of Lovastatin in Ethyl Acetate, Propyl Acetate, Isopropyl Acetate, Butyl Acetate, sec-Butyl Acetate, Isobutyl Acetate, tert-Butyl Acetate, and 2-Butanone between (285 and 323) K:	https://www.doi.org/10.1021/je800120p
Liquid–Liquid Equilibrium of the Ternary System Water + sec-Butyl Alcohol + sec-butyl acetate + N,N-dimethyl formamide at 101.3 kPa:	https://www.doi.org/10.1021/acs.jced.9b00103
Isobaric Vapor-Liquid Equilibrium for the Binary Systems of 1,2-Dichloroethane + sec-Butyl Acetate, n-Propyl Acetate, and tert-Butyl Acetate at 101.3 kPa:	https://www.doi.org/10.1016/j.fluid.2014.09.021
Experimental isobaric vapour-liquid equilibrium for ternary system of sec-butyl alcohol + sec-butyl acetate + N,N-dimethyl formamide at 101.3 kPa:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.doi.org/10.1021/acs.jced.8b00434
Experimental isobaric vapour-liquid equilibrium data for the binary system (N, N-dimethyl acetamide + dimethyl sulfoxide) and the quaternary system (sec-butyl acetate + sec-butyl alcohol + N, N-dimethyl acetamide + dimethyl sulfoxide) at 101.3 kPa:	https://www.chemeo.com/doc/models/crippen_log10ws
Isobaric Vapor-Liquid Equilibrium for the Binary Systems of sec-Butyl Acetate + Methyl Ethyl Ketone, 2-Methoxyethanol, or 1,2-Dimethoxyethane at 101.3 kPa:	https://www.doi.org/10.1016/j.jct.2019.05.005
	https://www.doi.org/10.1021/acs.jced.5b00582

Legend

cpg:	Ideal gas heat capacity
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume