Butyl lactate

Other names:	(S)-n-butyl lactate
	2-Hydroxypropanoic acid butyl ester
	Butyl «alpha»-hydroxypropionate
	Butylester kyseliny mlecne
	Lactic acid n-butyl ester
	NSC 6533
	butyl (S)-2-hydroxypropanoate
	butyl 2-hydroxypropanoate
	butyl L-(+)-lactate
	butyl L-lactate
	lactic acid, butyl ester
	n-Butyl lactate
	propanoic acid, 2-hydroxy-, butyl ester
Inchi:	InChI=1S/C7H14O3/c1-3-4-5-10-7(9)6(2)8/h6,8H,3-5H2,1-2H3
InchiKey:	MRABAEUHTLLEML-UHFFFAOYSA-N
Formula:	C7H14O3
SMILES:	CCCCOC(=O)C(C)O
Mol. weight [g/mol]:	146.18
CAS:	138-22-7

Physical Properties

Property code	Value	Unit	Source
gf	-365.12	kJ/mol	Joback Method
hf	-590.12	kJ/mol	Joback Method
hfus	17.24	kJ/mol	Joback Method
hvap	56.62	kJ/mol	Joback Method
log10ws	-0.99		Crippen Method
logp	0.710		Crippen Method
mcvol	122.800	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
rinpol	997.00		NIST Webbook
ripol	1520.00		NIST Webbook
ripol	1508.00		NIST Webbook
tb	459.20	K	NIST Webbook
tc	700.51	K	Joback Method
tf	245.00 ± 2.00	K	NIST Webbook
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.76	J/mol×K	527.59	Joback Method
cpg	298.85	J/mol×K	556.41	Joback Method
cpg	308.56	J/mol×K	585.23	Joback Method
cpg	317.88	J/mol×K	614.05	Joback Method
cpg	326.83	J/mol×K	642.87	Joback Method
cpg	335.40	J/mol×K	671.69	Joback Method
cpg	343.59	J/mol×K	700.51	Joback Method
dvisc	0.0172601	Pa×s	286.63	Joback Method
dvisc	0.0045782	Pa×s	326.79	Joback Method
dvisc	0.0016237	Pa×s	366.95	Joback Method
dvisc	0.0007065	Pa×s	407.11	Joback Method
dvisc	0.0003570	Pa×s	447.27	Joback Method
dvisc	0.0002019	Pa×s	487.43	Joback Method
dvisc	0.0001245	Pa×s	527.59	Joback Method
hvapt	49.90	kJ/mol	425.50	NIST Webbook
hvapt	58.70	kJ/mol	397.50	NIST Webbook
pvap	0.10	kPa	305.10	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.11	kPa	308.10	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods

pvap	0.13	kPa	308.50	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.15	kPa	311.00	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.07	kPa	302.20	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.19	kPa	314.50	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.23	kPa	317.00	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods

pvap	0.25	kPa	318.90	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods	
pvap	0.35	kPa	322.90	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods	
pvap	0.06	kPa	299.20	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods	
pvap	0.04	kPa	296.20	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods	
pvap	0.04	kPa	293.30	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods	

pvap	0.03	kPa	291.80	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.03	kPa	290.30	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.02	kPa	287.30	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.02	kPa	285.40	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.01	kPa	283.20	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods

pvap	0.01	kPa	281.80	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods	
pvap	0.01	kPa	280.70	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods	
pvap	9.96e-03	kPa	279.20	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods	
pvap	8.68e-03	kPa	277.20	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods	
pvap	8.23e-03	kPa	276.60	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods	

pvap	6.27e-03	kPa	274.10	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.16	kPa	313.00	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	5.76e-03	kPa	273.60	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
rfi	1.42180		293.15	Vapor liquid equilibria and excess volumes of the binary systems ethanol + ethyl lactate, isopropanol + isopropyl lactate and n-butanol + n-butyl lactate at 101.325 kPa
rhol	967.57	kg/m3	308.15	Experimental measurements and modelling of volumetric properties, refractive index and viscosity of selected binary systems with butyl lactate at 288.15 to 323.15 K and atmospheric pressure. New UNIFAC-VISCO interaction parameters.

rhol	972.51	kg/m3	303.15	Experimental measurements and modelling of volumetric properties, refractive index and viscosity of selected binary systems with butyl lactate at 288.15 to 323.15 K and atmospheric pressure. New UNIFAC-VISCO interaction parameters.	
rhol	952.63	kg/m3	323.15	Experimental measurements and modelling of volumetric properties, refractive index and viscosity of selected binary systems with butyl lactate at 288.15 to 323.15 K and atmospheric pressure. New UNIFAC-VISCO interaction parameters.	
rhol	996.90	kg/m3	278.15	Thermophysical Properties of Lactates	
rhol	994.47	kg/m3	280.65	Thermophysical Properties of Lactates	
rhol	992.02	kg/m3	283.15	Thermophysical Properties of Lactates	
rhol	989.58	kg/m3	285.65	Thermophysical Properties of Lactates	
rhol	987.13	kg/m3	288.15	Thermophysical Properties of Lactates	
rhol	984.67	kg/m3	290.65	Thermophysical Properties of Lactates	
rhol	982.21	kg/m3	293.15	Thermophysical Properties of Lactates	
rhol	979.75	kg/m3	295.65	Thermophysical Properties of Lactates	
rhol	977.28	kg/m3	298.15	Thermophysical Properties of Lactates	

rhol	974.81	kg/m3	300.65	Thermophysical Properties of Lactates
rhol	972.34	kg/m3	303.15	Thermophysical Properties of Lactates
rhol	969.86	kg/m3	305.65	Thermophysical Properties of Lactates
rhol	967.37	kg/m3	308.15	Thermophysical Properties of Lactates
rhol	964.89	kg/m3	310.65	Thermophysical Properties of Lactates
rhol	962.40	kg/m3	313.15	Thermophysical Properties of Lactates
rhol	959.90	kg/m3	315.65	Thermophysical Properties of Lactates
rhol	957.41	kg/m3	318.15	Thermophysical Properties of Lactates
rhol	954.91	kg/m3	320.65	Thermophysical Properties of Lactates
rhol	952.41	kg/m3	323.15	Thermophysical Properties of Lactates
rhol	949.90	kg/m3	325.65	Thermophysical Properties of Lactates
rhol	947.40	kg/m3	328.15	Thermophysical Properties of Lactates
rhol	944.88	kg/m3	330.65	Thermophysical Properties of Lactates
rhol	942.37	kg/m3	333.15	Thermophysical Properties of Lactates
rhol	939.85	kg/m3	335.65	Thermophysical Properties of Lactates
rhol	937.32	kg/m3	338.15	Thermophysical Properties of Lactates
rhol	982.00	kg/m3	293.15	Investigation of the Solubilities of Carbon Dioxide in Some Low Volatile Solvents and Their Thermodynamic Properties

rhol	977.45	kg/m3	298.15	Experimental measurements and modelling of volumetric properties, refractive index and viscosity of selected binary systems with butyl lactate at 288.15 to 323.15 K and atmospheric pressure. New UNIFAC-VISCO interaction parameters.	
rhol	982.37	kg/m3	293.15	Experimental measurements and modelling of volumetric properties, refractive index and viscosity of selected binary systems with butyl lactate at 288.15 to 323.15 K and atmospheric pressure. New UNIFAC-VISCO interaction parameters.	
rhol	987.27	kg/m3	288.15	Experimental measurements and modelling of volumetric properties, refractive index and viscosity of selected binary systems with butyl lactate at 288.15 to 323.15 K and atmospheric pressure. New UNIFAC-VISCO interaction parameters.	
rhol	940.10	kg/m3	338.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties	
rhol	944.10	kg/m3	333.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties	

rhol	948.90	kg/m3	328.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	953.90	kg/m3	323.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	958.50	kg/m3	318.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	963.50	kg/m3	313.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	968.40	kg/m3	308.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	973.10	kg/m3	303.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	977.00	kg/m3	298.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	981.50	kg/m3	293.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	977.28	kg/m3	298.15	Self-aggregation of liquids from biomass in aqueous solution

rhol	962.60	kg/m3	313.15	Experimental measurements and modelling of volumetric properties, refractive index and viscosity of selected binary systems with butyl lactate at 288.15 to 323.15 K and atmospheric pressure. New UNIFAC-VISCO interaction parameters.	
rhol	957.62	kg/m3	318.15	Experimental measurements and modelling of volumetric properties, refractive index and viscosity of selected binary systems with butyl lactate at 288.15 to 323.15 K and atmospheric pressure. New UNIFAC-VISCO interaction parameters.	

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
283.15	100.00	992.75
288.15	100.00	987.86
293.15	100.00	982.96
298.15	100.00	977.96
303.15	100.00	973.09
308.15	100.00	967.74
313.15	100.00	963.05
318.15	100.00	957.98
323.15	100.00	952.44
328.15	100.00	947.31

333.15	100.00	942.28
338.15	100.00	937.09
283.15	2500.00	994.4
288.15	2500.00	989.52
293.15	2500.00	984.69
298.15	2500.00	979.83
303.15	2500.00	974.98
308.15	2500.00	970.01
313.15	2500.00	965.11
318.15	2500.00	960.06
323.15	2500.00	954.61
328.15	2500.00	949.44
333.15	2500.00	944.52
338.15	2500.00	939.39
283.15	5000.00	996.14
288.15	5000.00	991.32
293.15	5000.00	986.5
298.15	5000.00	981.74
303.15	5000.00	976.81
308.15	5000.00	971.95
313.15	5000.00	967.03
318.15	5000.00	962.11
323.15	5000.00	956.73
328.15	5000.00	951.63
333.15	5000.00	946.72
338.15	5000.00	941.78
283.15	7500.00	997.77
288.15	7500.00	993.09
293.15	7500.00	988.29
298.15	7500.00	983.49
303.15	7500.00	978.72
308.15	7500.00	973.85
313.15	7500.00	969.06
318.15	7500.00	964.16
323.15	7500.00	958.74
328.15	7500.00	953.79
333.15	7500.00	948.91
338.15	7500.00	943.99
283.15	10000.00	999.41
288.15	10000.00	994.7
293.15	10000.00	990.02
298.15	10000.00	985.26
303.15	10000.00	980.54
308.15	10000.00	975.59

313.15	10000.00	970.96
318.15	10000.00	966.04
323.15	10000.00	960.79
328.15	10000.00	955.86
333.15	10000.00	951.02
338.15	10000.00	946.05
283.15	20000.00	1005.87
288.15	20000.00	1001.18
293.15	20000.00	996.69
298.15	20000.00	992.04
303.15	20000.00	987.67
308.15	20000.00	982.84
313.15	20000.00	978.27
318.15	20000.00	973.62
323.15	20000.00	968.64
328.15	20000.00	963.73
333.15	20000.00	959.28
338.15	20000.00	954.42
283.15	30000.00	1011.69
288.15	30000.00	1007.12
293.15	30000.00	1002.96
298.15	30000.00	998.37
303.15	30000.00	993.96
308.15	30000.00	989.43
313.15	30000.00	985.03
318.15	30000.00	980.42
323.15	30000.00	975.86
328.15	30000.00	971.08
333.15	30000.00	966.7
338.15	30000.00	962.07
283.15	40000.00	1017.42
288.15	40000.00	1012.83
293.15	40000.00	1008.73
298.15	40000.00	1004.29
303.15	40000.00	1000.06
308.15	40000.00	995.62
313.15	40000.00	991.43
318.15	40000.00	986.96
323.15	40000.00	982.37
328.15	40000.00	977.8
333.15	40000.00	973.8
338.15	40000.00	969.19
283.15	50000.00	1022.85
288.15	50000.00	1018.14

293.15	50000.00	1014.33
298.15	50000.00	1009.82
303.15	50000.00	1005.69
308.15	50000.00	1001.41
313.15	50000.00	997.35
318.15	50000.00	993.12
323.15	50000.00	988.47
328.15	50000.00	984.21
333.15	50000.00	980.2
338.15	50000.00	975.64
283.15	60000.00	1027.71
288.15	60000.00	1023.26
293.15	60000.00	1019.37
298.15	60000.00	1015.17
303.15	60000.00	1011.27
308.15	60000.00	1007.05
313.15	60000.00	1002.99
318.15	60000.00	998.83
323.15	60000.00	994.3
328.15	60000.00	990.17
333.15	60000.00	986.43
338.15	60000.00	982.05

Reference *https://www.doi.org/10.1016/j.jct.2012.11.002*

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor liquid equilibria and excess volumes of the binary systems ethanol + ethyl lactate, isopropanol + isopropyl lactate and n-butanol + n-butyl lactate at 101.325 kPa:	https://www.doi.org/10.1016/j.fluid.2005.02.015
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C138227&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Feasibility of bio-based lactate esters as extractant for biobutanol recovery: (Liquid + liquid) equilibria:	https://www.doi.org/10.1016/j.jct.2015.10.003
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
High-pressure phase behavior of propyl lactate and butyl lactate in supercritical carbon dioxide:	https://www.doi.org/10.1016/j.jct.2011.10.010
Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties:	https://www.doi.org/10.1016/j.jct.2017.12.021
Renewable platform chemicals:	https://www.doi.org/10.1016/j.jct.2018.07.029
Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods:	https://www.doi.org/10.1016/j.tca.2013.03.025
Experimental measurements and modelling of volumetric properties, speed of sound and refractive index and viscosity of selected binary systems with butyl lactate at 288.15 to 323.15 K and atmospheric pressure. New UNIFAC-VISCO interaction parameters.:	https://www.doi.org/10.1016/j.tca.2013.11.010
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Self-aggregation of liquids from biomass in aqueous solution:	https://www.doi.org/10.1016/j.jct.2013.06.020
The pqT behaviour of the lactate family:	https://www.doi.org/10.1016/j.jct.2012.11.002

Investigation of the Solubilities of Carbon Dioxide in Some Low Volatile Solvents and Their Thermodynamic Properties: https://www.doi.org/10.1021/acs.jced.5b00893

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
hvapt:	Enthalpy of vaporization at a given temperature
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