J. Chem. Thermodynamics 58 (2013) 8–13

Contents lists available at SciVerse ScienceDirect

J. Chem. Thermodynamics

journal homepage: www.elsevier.com/locate/jct

The $p\rho T$ behaviour of the lactate family

Laura Lomba [a], Mª Rosa Pino [a], Carlos Lafuente [b], Mª Carmen Lopez [b], Beatriz Giner [a,*]

[a] Facultad de Ciencias de la Salud, Universidad San Jorge, Villanueva de Gállego, 50830 Zaragoza, Spain
[b] Departamento de Química Física, Facultad de Ciencias, Universidad de Zaragoza, 50009 Zaragoza, Spain

ARTICLE INFO

Article history:
Received 11 September 2012
Received in revised form 31 October 2012
Accepted 2 November 2012
Available online 10 November 2012

Keywords:
Methyl lactate
Ethyl lactate
Butyl lactate
Density
Pressure

ABSTRACT

The densities of methyl lactate, ethyl lactate and butyl lactate have been measured using a high-pressure, high-temperature vibrating tube densimeter system over a temperature range from $T = (283.15$ to $338.15)$ K and a pressure range from $p = (0.1$ to $60.0)$ MPa. The experimental densities have been satisfactorily correlated with temperature and pressure using the TRIDEN equation. Finally, from the experimental densities, properties such as isobaric expansibility and isothermal compressibility have been calculated.

1. Introduction

Nowadays, it is a well-known fact that one of the most important challenges for the chemical industry is that of reducing pollution as much as possible. Perhaps, the most effective way to achieve this is through changing solvents used in industrial processes. The solvents that are now currently in use are the basis of our chemical operations and most of them are still organic products derived from petroleum and are widely used in much of our solution chemistry and separation issues. However, these kinds of solvents can cause health and environmental problems which should be prevented [1].

Therefore, there is a need to develop "greener" organic solvents that can maintain a sustainable environment. This can be achieved in two different ways, firstly through renewable feedstock, and secondly by understanding the relationship between the structure and toxicity of chemicals, this second form is more difficult to obtain, but it allows for modification in the design of chemicals in order to reduce their environmental impact [2,3].

Organic esters, which are a very important class of chemicals with applications in a wide range of areas in the chemical industry, such as perfumes, flavourings, pharmaceuticals, plasticizers, solvents and intermediates are some of the above-mentioned greener solvents. An important family within this kind is the lactate family. It should be mentioned that ethyl lactate has attracted much attention in recent years and we now have some important data on these chemicals. Some industry experts suggest that ethyl lactate could replace traditional solvents in more than 80% of their applications. However, this is perhaps an exaggeration; since ethyl lactate has a high boiling polar and it is a protic solvent, meaning that it cannot be used for applications when non-polar, aprotic and/or lower boiling point solvents are required [4].

It is also surprising, that despite their potential applications, no in depth studies have been carried out on chemicals from the lactate family from a thermophysical perspective. Several properties for ethyl lactate have been measured such as density, viscosity, refractive index or $p\rho T$ behaviour, [4,5] however, it is possible to expand the existing information on this family as they could be used as solvents in the future for different industries. Therefore, in this paper, we would like to pay special attention to the volumetric behaviour of some lactate family chemicals.

The selected solvents studied are methyl lactate (methyl 2-hydroxypropionate, CAS number 547-64-8), ethyl lactate (ethyl 2-hydroxypropionate, CAS number 97-64-3) and butyl lactate (butyl 2-hydroxypropionate, CAS number 138-22-7) obtained from Aldrich. All of these compounds are derived from lactic acid which can be produced either from chemical synthesis or through the fermentation of different carbohydrates, such as, glucose (from starch), lactose (from whey), maltose (produced by specific enzymatic starch conversion) or sucrose (from syrups, juices, and molasses) [6,7].

The $p\rho T$ study was carried out over a temperature range from $T = (283.15$ to $338.15)$ K and a pressure range from $p = (0.1$ to $60.0)$ MPa for all of the chemicals studied. Experimental density data were fitted to the TRIDEN and from the fitted equation, related

* Corresponding author. Tel.: +34 976 060100.
E-mail address: bginer@usj.es (B. Giner).

0021-9614/$ - see front matter © 2012 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.jct.2012.11.002

TABLE 1
Provenance and purity of the materials studied.

Chemical name	Source	Initial mass fraction purity	Final mass fraction purity
Methyl lactate	TCI	0.98	0.98
Ethyl lactate	Sigma–Aldrich	0.98	0.98
Butyl lactate	Sigma–Aldrich	0.98	0.98

TABLE 2
Volumetric properties at $T = 298.15$ K and $p = 0.1$ MPa and comparison of experimental densities with literature density values.[a]

Compound	$\rho^{exptl}/(kg \cdot m^{-3})$	$\rho^{lit}/(kg \cdot m^{-3})$	α_p/kK^{-1}	κ_T/TPa^{-1}
Methyl lactate	1087.76		1.0283	655.86
Ethyl lactate	1028.78	1028.3[5] 1028.6[13] 1028.9[14]	1.0606	757.60
Butyl lactate	977.96		1.0187	780.70

[a] Standard uncertainties u are $u(T) = 0.01$ K, $u(p) = 0.005$ MPa, and the combined expanded uncertainty U_c is $U_c(\rho) = 0.1$ kg · m^{-3} with 0.95 level of confidence ($k \approx 2$).

properties, such as isobaric thermal expansion, α, and isothermal compressibility, k_T, have been obtained.

TABLE 4
Parameters of the TRIDEN equation and relative root-mean-square deviations, *RMSDr*, between experimental and correlated densities.

	Methyl lactate	Ethyl lactate	Butyl lactate
$A_R/(kg \cdot m^{-3})$	468.51	163.33	409.68
B_R	0.5789	0.351	0.57323
C_R/K	480.4627	600.1200	480.08731
D_R	0.63402	0.40374	0.59092
C_T	0.07652	0.07853	0.07903
b_o/MPa	314.7917	272.0701	177.89984
b_1/MPa	15.73594	15.47006	82.36898
b_2/MPa	−35.91014	−32.47918	−47.19416
b_3/MPa	4.47645	4.05772	5.15696
E_T/K	83.3801	85.6665	81.90837
RMSDr/%	0.00601	0.00650	0.016340

2. Experimental

Information on the racemic liquids used is summarized in table 1. All compounds were used without further purification because the impurities are of such a low concentration that the physical properties are almost unaffected within the quoted uncertainty of the measurements [8].

Densities were measured using a high pressure, high temperature Anton Paar DMA HP cell connected to an Anton Paar DMA 5000 evaluation unit. The density of the sample was determined

TABLE 3
Experimental densities, ρ, as a function of temperature and pressure.[a]

T/K	$\rho/(kg \cdot m^{-3})$ at p/MPa									
	0.1	2.5	5.0	7.5	10.0	20.0	30.0	40.0	50.0	60.0
					Methyl lactate					
283.15	1104.41	1106.00	1107.57	1109.14	1110.68	1116.59	1122.23	1127.45	1132.48	1137.40
288.15	1098.86	1100.48	1102.13	1103.77	1105.31	1111.55	1117.27	1122.78	1127.98	1132.78
293.15	1093.31	1094.99	1096.72	1098.35	1099.92	1106.20	1112.08	1117.65	1122.93	1128.01
298.15	1087.76	1089.42	1091.21	1092.88	1094.57	1101.03	1107.23	1112.83	1118.24	1123.43
303.15	1082.13	1083.92	1085.75	1087.50	1089.23	1095.82	1101.97	1107.90	1113.44	1118.66
308.15	1076.53	1078.32	1080.19	1082.00	1083.79	1090.68	1097.03	1102.99	1108.63	1114.02
313.15	1070.85	1072.76	1074.65	1076.52	1078.39	1085.28	1091.84	1097.99	1103.74	1109.24
318.15	1065.11	1067.04	1068.97	1070.94	1072.77	1080.09	1086.77	1093.08	1098.93	1104.49
323.15	1059.39	1061.40	1063.43	1065.44	1067.34	1074.67	1081.41	1088.00	1094.04	1099.76
328.15	1053.63	1055.70	1057.77	1059.74	1061.80	1069.41	1076.50	1083.15	1089.40	1095.07
333.15	1047.83	1049.97	1052.16	1054.23	1056.23	1064.05	1071.33	1078.01	1084.39	1090.37
338.15	1042.00	1044.15	1046.35	1048.52	1050.63	1058.63	1066.13	1073.12	1079.74	1085.76
					Ethyl lactate					
283.15	1045.06	1046.77	1048.51	1050.24	1051.88	1058.39	1064.45	1070.13	1075.50	1080.55
288.15	1039.64	1041.39	1043.21	1044.99	1046.74	1053.28	1059.46	1065.24	1070.74	1076.04
293.15	1034.25	1036.05	1037.86	1039.70	1041.50	1048.30	1054.58	1060.54	1066.26	1071.55
298.15	1028.78	1030.66	1032.56	1034.43	1036.23	1043.21	1049.76	1055.69	1061.53	1066.96
303.15	1023.32	1025.21	1027.24	1029.11	1031.00	1038.26	1044.91	1051.19	1056.95	1062.52
308.15	1017.84	1019.82	1021.87	1023.84	1025.70	1033.08	1039.92	1046.28	1052.19	1057.98
313.15	1012.33	1014.31	1016.42	1018.41	1020.39	1027.93	1034.97	1041.52	1047.69	1053.46
318.15	1006.72	1008.86	1011.01	1013.10	1015.13	1022.87	1030.04	1036.74	1042.96	1048.96
323.15	1001.23	1003.36	1005.56	1007.68	1009.78	1017.76	1025.13	1031.99	1038.42	1044.49
328.15	995.54	997.80	1000.11	1002.34	1004.46	1012.65	1020.17	1027.16	1033.75	1039.99
333.15	989.91	992.19	994.55	996.87	999.06	1007.62	1015.40	1022.50	1029.24	1035.71
338.15	984.30	986.71	989.18	991.49	993.65	1002.34	1010.27	1017.75	1024.55	1031.04
					Butyl lactate					
283.15	992.75	994.40	996.14	997.77	999.41	1005.87	1011.69	1017.42	1022.85	1027.71
288.15	987.86	989.52	991.32	993.09	994.70	1001.18	1007.12	1012.83	1018.14	1023.26
293.15	982.96	984.69	986.50	988.29	990.02	996.69	1002.96	1008.73	1014.33	1019.37
298.15	977.96	979.83	981.74	983.49	985.26	992.04	998.37	1004.29	1009.82	1015.17
303.15	973.09	974.98	976.81	978.72	980.54	987.67	993.96	1000.06	1005.69	1011.27
308.15	967.74	970.01	971.95	973.85	975.59	982.84	989.43	995.62	1001.41	1007.05
313.15	963.05	965.11	967.03	969.06	970.96	978.27	985.03	991.43	997.35	1002.99
318.15	957.98	960.06	962.11	964.16	966.04	973.62	980.42	986.96	993.12	998.83
323.15	952.44	954.61	956.73	958.74	960.79	968.64	975.86	982.37	988.47	994.30
328.15	947.31	949.44	951.63	953.79	955.86	963.73	971.08	977.80	984.21	990.17
333.15	942.28	944.52	946.72	948.91	951.02	959.28	966.70	973.80	980.20	986.43
338.15	937.09	939.39	941.78	943.99	946.05	954.42	962.07	969.19	975.64	982.05

[a] Standard uncertainties u are $u(T) = 0.01$ K, $u(p) = 0.005$ MPa, and the combined expanded uncertainty U_c is $U_c(\rho) = 0.1$ kg · m^{-3} with 0.95 level of confidence ($k \approx 2$).