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NOMENCLATURE

A, B, C = Antoine constants
DMB = 2,3-dimethylbutane
mm. = millimeters
P = pressure, in mm. of Hg
R = gas constant
T = temperature, absolute
t = temperature, °C.
x_{i_c} = calculated mole fraction of component i in the liquid phase
x_{i_e} = experimental mole fraction of component i in the liquid phase
y_{i_c} = calculated mole fraction of component i in the vapor phase
y_{i_e} = experimental fraction of component i in the vapor phase
α_{ij} = relative volatility of component i to component j
$(\lambda_{ij} - \lambda_{ii})$, $(\lambda_{ji} - \lambda_{jj})$ = empirically determined Wilson parameter energy terms (for constant pressure data here) related to the cohesive energy density, and appearing in the Wilson equation, Equations 3; cal. per gram-mole
Λ_{ij}, Λ_{ji} = dimensionless expression in Wilson equation, defined in Equations 3
γ = activity coefficient

Subscripts

A = acetone
c = calculated
C = chloroform
D = 2,3-dimethylbutane
e = experimental
i, j, k = components i, j, k

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Vapor-Liquid Equilibrium of the System 2-Propanol–Water–1,2,3-Propanetriol at 760 Mm. of Hg

LUCIEN VERHOEYE and EDDY LAUWERS
Laboratory of Organic Industrial Chemistry and Chemical Engineering,
State University of Ghent, J. Plateaustraat, 22, Ghent, Belgium

The vapor-liquid equilibrium data of the ternary system 2-propanol–water–1,2,3-propanetriol for 1,2,3-propanetriol contents of 10, 20, 30, 40, and 50 wt. % have been reported. A diagram containing lines of constant value of specific gravity d_{25}^{25} and refractive index n_D^{25} has also been reported.

VAPOR-LIQUID equilibrium data of the ternary system 2-propanol-water-1,2,3-propanetriol have been determined by means of an Othmer still (*4*). The samples were analyzed by determination of refractive index and specific gravity. These data were not published for the ternary system or for the binary system, 2-propanol-1,2,3-propanetriol. Consequently, they are published in the present paper, and a diagram containing lines of constant value of specific gravity and refractive index is also added.

EXPERIMENTAL

Purity of Materials. The purification of 2-propanol was carried out by rectification through a glass column 3 cm. in diameter and 2 meters high, containing packings of 3 mm. in stainless steel wire, under high reflux.

The purification of 1,2,3-propanetriol was carried out by distillation at reduced pressure of about 10 mm. of Hg through a well-insulated 1-meter-high Vigreux column.

A large quantity of starting material was used and many fractions were sampled. Only the fractions of which the specific gravity and the refractive index remain constant were kept. The physical properties of the materials used in the present work are listed and compared with critically chosen values from literature in Table I.

Table I. Physical Properties of Materials

	Specific Gravity, d_4^{25}		Refractive Index, n_D^{25}	
Materials	Exptl.	Lit. (6)	Exptl.	Lit. (6)
1,2,3-propanetriol	1.2581	1.25822[a]	1.4732	1.47352
2-Propanol	0.7808	0.78095	1.3749	1.3747

[a] Interpolated.

Analytical Method. Analysis was carried out by measurement of specific gravity and refractive index. More sets of data of these properties for the systems 2-propanol-water and water–1,2,3-propanetriol have been published (*3*, *5*).

Experimental check of the data listed by Hatch (*3*) for the system 2-propanol-water proves that they are sufficiently accurate. Specific gravity data by Bosart and Snoddy and refractive index data by Iyher and Usher, both compiled by Timmermans (*5*) for the system water–1,2,3-propanetriol, also agree sufficiently with our checks. These data have been used in the present study, and consequently, no data for these systems have been listed.

Table II. Specific Gravity and Refractive Index of Mixtures of the System 2-Propanol–1,2,3-Propanetriol

1,2,3-Propanetriol, Wt. %	Specific Gravity, d_{25}^{25}	Refractive Index, n_D^{25}
5.02	0.7995	1.3788
10.12	0.8165	1.3829
16.91	0.8406	1.3881
23.03	0.8635	1.3931
29.89	0.8902	1.3991
39.86	0.9328	1.4082
45.59	0.9568	1.4140
48.20	0.9626	1.4164
49.91	0.9763	1.4182
52.91	0.9911	1.4208
56.02	1.0064	1.4245
59.06	1.0214	1.4271
70.17	1.0797	1.4370
80.07	1.1396	1.4513
85.10	1.1672	1.4576
89.20	1.1925	1.4617

Data of refractive index and specific gravity of the system 2-propanol–1,2,3-propanetriol are listed in Table II.

Different sets of mixtures of known composition are prepared in this way, so that the whole composition range of the ternary system is covered. Each set contains a constant content of water and different contents of the other compounds. The sets are prepared at intervals of 10 wt. % of water. The refractive index and the specific gravity of these mixtures are listed in Table III.

A chart (Figure 1) containing lines of constant value of specific gravity and refractive index is derived from these data by the following graphical method. By plotting the physical property against the per cent of most volatile compound for each set of constant water content, a chart (not reproduced here) containing a set of curves corresponding to the different contents of water is obtained. From this chart the composition of mixtures corresponding to a fixed value of the physical property can be derived.

The measurements of the refractive index are made by an Abbe refractometer with an accuracy of ±0.0002, and

Table III. Specific Gravity and Refractive Index of Ternary Mixtures of the System 2-Propanol–Water–1,2,3-Propanetriol

Composition			
Water, wt. %	1,2,3-Propanetriol, wt. %	Specific Gravity, d_{25}^{25}	Refractive Index, n_D^{25}
90.0	4.94	1.0027	1.3429
90.0	10.00	1.0245	1.3451
80.0	4.94	0.9878	1.3520
80.0	9.93	1.0069	1.3536
80.0	14.96	1.0268	1.3553
70.0	4.94	0.9704	1.3601
70.0	9.99	0.9909	1.3622
70.0	14.99	1.0109	1.3641
70.0	20.15	1.0319	1.3662
70.0	24.96	1.0516	1.3680
60.0	9.99	0.9690	1.3687
60.0	15.96	0.9903	1.3718
60.0	19.99	1.0120	1.3741
60.0	24.95	1.0334	1.3768
60.0	30.00	1.0553	1.3790
60.0	35.17	1.0779	1.3812
50.0	9.97	0.9448	1.3732
50.0	14.97	0.9655	1.3768
50.0	20.02	0.9877	1.3799
50.0	25.09	1.0105	1.3832
50.0	30.06	1.0334	1.3864
50.0	35.00	1.0562	1.3895
50.0	40.00	1.0797	1.3924
50.0	44.97	1.1030	1.3951
40.0	4.48	0.8985	1.3736
40.0	9.95	0.9202	1.3771
40.0	14.47	0.9375	1.3802
40.0	19.94	0.9618	1.3841
40.0	24.91	0.9827	1.3878
40.0	29.83	1.0063	1.3912
40.0	34.94	1.0293	1.3952
40.0	39.96	1.0546	1.3989
40.0	45.00	1.0786	1.4026
40.0	50.03	1.1039	1.4060
40.0	54.97	1.1286	1.4091
30.0	5.03	0.8748	1.3767
30.0	9.82	0.8931	1.3799
30.0	14.92	0.9133	1.3837
30.0	20.04	0.9342	1.3875
30.0	24.88	0.9551	1.3912
30.0	29.95	0.9770	1.3951
30.0	34.99	1.0009	1.3991
30.0	39.92	1.0246	1.4031
30.0	44.94	1.0494	1.4072
30.0	49.78	1.0746	1.4113
30.0	55.02	1.1014	1.4159
30.0	59.99	1.1279	1.4199
30.0	65.00	1.1548	1.4247
20.0	4.97	0.8499	1.3783
20.0	9.80	0.8676	1.3819
20.0	14.92	0.8872	1.3858
20.0	20.05	0.9076	1.3897
20.0	24.93	0.9277	1.3934
20.0	29.99	0.9491	1.3975
20.0	34.97	0.9715	1.4019
20.0	39.70	0.9933	1.4060
20.0	44.72	1.0172	1.4110
20.0	49.77	1.0424	1.4190
20.0	55.02	1.0693	1.4200
20.0	60.05	1.0958	1.4245
20.0	64.94	1.1231	1.4290
20.0	70.01	1.1518	1.4339
20.0	75.00	1.1802	1.4380
10.0	5.01	0.8245	1.3794
10.0	9.97	0.8423	1.3829
10.0	15.06	0.8597	1.3868
10.0	19.85	0.8790	1.3906
10.0	25.00	0.9000	1.3968
10.0	29.97	0.9196	1.3991
10.0	34.89	0.9412	1.4052
10.0	39.79	0.9623	1.4077
10.0	45.00	0.9872	1.4141
10.0	49.95	1.0100	1.4172
10.0	54.74	1.0346	1.4234
10.0	58.81	1.0551	1.4259
10.0	64.96	1.0886	1.4347
10.0	69.96	1.1163	1.4374
10.0	79.98	1.1753	1.4478
10.0	84.51	1.2010	1.4538

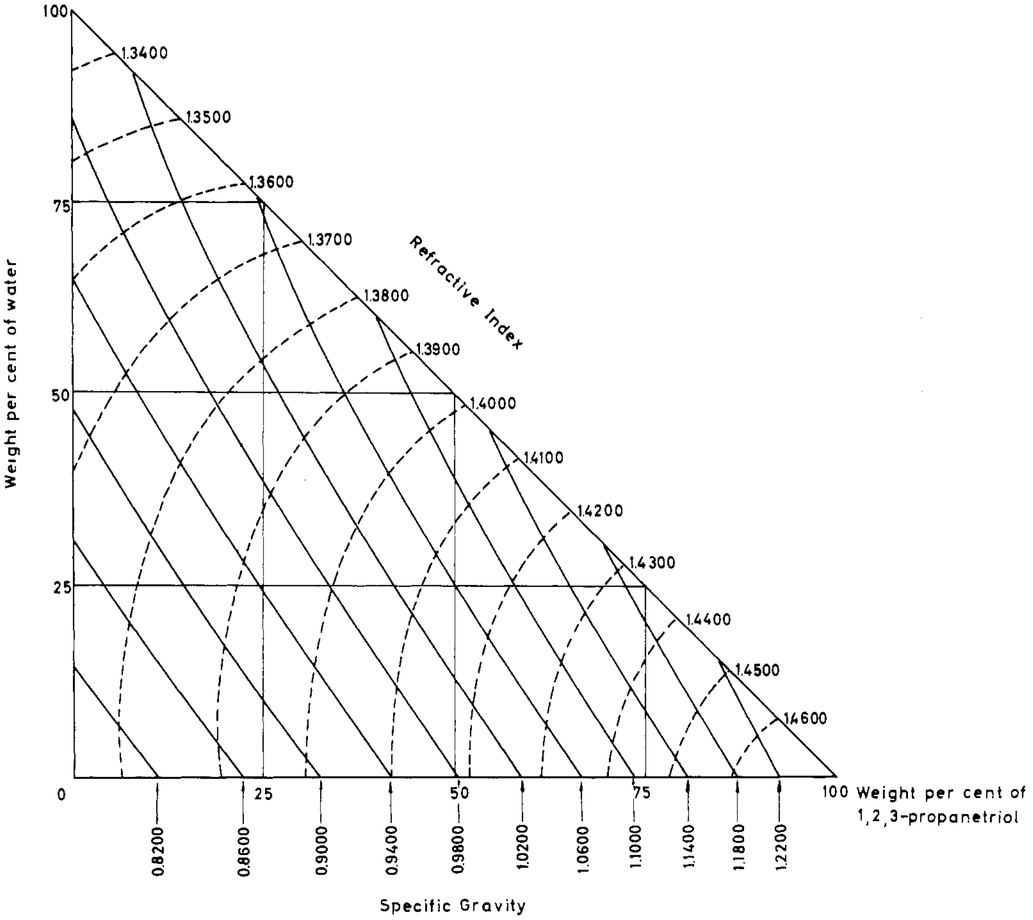

Figure 1. Analysis diagram

— Lines of constant specific gravity

--- Lines of constant refractive index

the measurements of the specific gravity with an accuracy of ±0.0001. The temperature was kept constant at 25.0 ± 0.1° C.

The determination of water in 1,2,3-propanetriol (*2*) and in mixtures of 1,2,3-propanetriol and 2-propanol can be carried out by the Karl Fischer titration method. The relative error of this analysis is about 1%. For low water contents, it was more accurate to carry out the analysis by measurement of one physical constant and titration of water. For mixtures with higher water contents, the analysis was carried out by measurement of two physical properties. The accuracy is a function of the angle of intersection of the lines of constant refractive index and of constant specific gravity, which is for this system favorable in the whole concentration range.

Determination of Vapor-Liquid Equilibrium Data. An Othmer still (*4*) was used for the determination of the vapor-liquid equilibrium. Partial condensation in the upper part of the still was avoided by applying an external heater, which kept the temperature of the space between the tube transporting the vapor to the condensor and the external wall a little higher than the temperature of the boiling liquid. Concentration gradients in the boiling liquid, arising by the flowing back of liquid from the condensate receiver in the vessel, were avoided by slow distillation and thorough stirring. The pressure was kept constant at 760 ± 0.5 mm. of Hg by means of a sulfuric acid manostat.

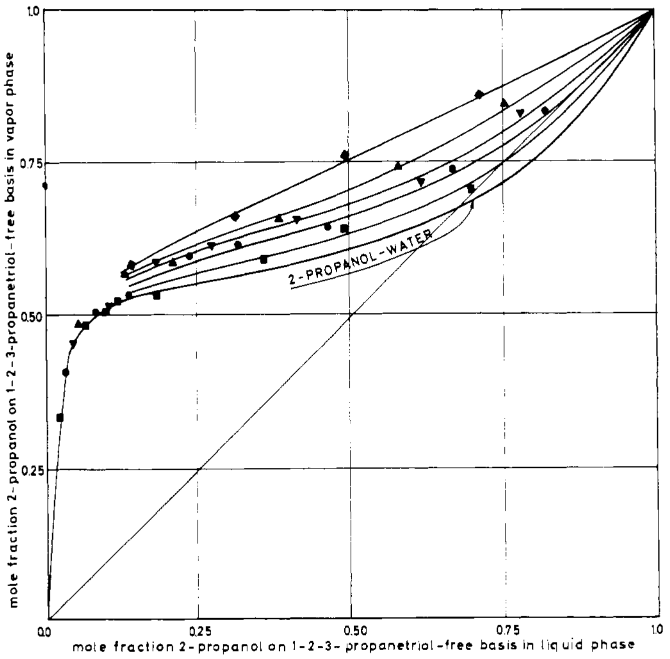

Figure 2. Vapor-liquid equilibrium diagram

■ Lines of 10 wt. % 1,2,3-propanetriol

● Lines of 20 wt. % 1,2,3-propanetriol

▼ Lines of 30 wt. % 1,2,3-propanetriol

▲ Lines of 40 wt. % 1,2,3-propanetriol

◆ Lines of 50 wt. % 1,2,3-propanetriol

RESULTS

There was good agreement for the whole concentration range between the present measurements and the data of

Table IV. Vapor-Liquid Equilibrium Data of the System 2-Propanol (*A*)–Water (*B*)–1,2,3-Propanetriol (C)

Temp., °C.	Mole Fraction in Liquid Phase		Mole Fraction in Vapor Phase		On 1,2,3-Propanetriol-Free Basis	
	2-Propanol	Water	2-Propanol	Water	Mole fraction of 2-propanol in liquid phase	Mole fraction of 2-propanol in vapor phase
			10 Wt. % 1,2,3-Propanetriol			
91.5	0.022	0.955	0.336	0.664	0.023	0.336
85.5	0.063	0.910	0.480	0.519	0.065	0.480
84.3	0.100	0.872	0.507	0.491	0.103	0.508
83.9	0.114	0.858	0.523	0.476	0.117	0.523
82.8	0.173	0.795	0.529	0.469	0.179	0.530
82.2	0.344	0.616	0.583	0.414	0.358	0.585
81.7	0.467	0.487	0.633	0.367	0.489	0.632
81.6	0.655	0.288	0.701	0.297	0.695	0.702
			20 Wt. % 1,2,3-Propanetriol			
90.1	0.031	0.915	0.407	0.591	0.033	0.407
85.1	0.077	0.867	0.505	0.494	0.081	0.506
83.8	0.129	0.808	0.533	0.468	0.139	0.532
83.1	0.198	0.729	0.582	0.418	0.213	0.582
83.0	0.202	0.729	0.596	0.405	0.233	0.596
82.7	0.290	0.632	0.610	0.388	0.315	0.611
82.6	0.419	0.487	0.640	0.359	0.463	0.640
83.0	0.592	0.294	0.738	0.262	0.669	0.735
			30 Wt. % 1,2,3-Propanetriol			
89.0	0.042	0.873	0.451	0.548	0.046	0.451
86.2	0.092	0.814	0.517	0.482	0.102	0.517
84.0	0.159	0.734	0.582	0.418	0.178	0.582
83.6	0.241	0.635	0.605	0.395	0.275	0.605
83.4	0.354	0.503	0.652	0.347	0.412	0.652
83.7	0.511	0.318	0.716	0.283	0.616	0.716
84.8	0.628	0.177	0.837	0.163	0.780	0.837
			40 Wt. % 1,2,3-Propanetriol			
89.9	0.047	0.822	0.436	0.564	0.054	0.436
87.3	0.111	0.743	0.571	0.426	0.130	0.573
85.0	0.172	0.651	0.580	0.419	0.209	0.580
84.5	0.306	0.492	0.656	0.342	0.384	0.657
85.0	0.438	0.321	0.743	0.258	0.577	0.743
85.9	0.548	0.182	0.845	0.155	0.751	0.845
			50 Wt. % 1,2,3-Propanetriol			
91.6	0.050	0.757	0.446	0.554	0.062	0.446
87.3	0.109	0.664	0.578	0.420	0.141	0.580
85.7	0.230	0.509	0.659	0.339	0.311	0.660
86.0	0.344	0.355	0.763	0.237	0.492	0.763
87.0	0.465	0.191	0.859	0.201	0.709	0.859

Brunjes and Bogart (*1*) for the system 2-propanol–water. Consequently, vapor-liquid equilibrium data of this system are not listed.

No 1,2,3-propanetriol was found in the vapor in equilibrium with liquid phases of the system water–1,2,3-propanetriol containing less than 80 wt. % of 1,2,3-propanetriol, and only small quantities above this concentration—e.g., 0.3 wt. % for 90 wt. % of 1,2,3-propanetriol in the liquid. Likewise, no 1,2,3-propanetriol was found in the vapor in equilibrium with liquid phases of the system 2-propanol–1,2,3-propanetriol containing less than 60 wt. % of 1,2,3-propanetriol, and only small quantities above this concentration—e.g., 0.2 wt. % for 80 wt. % of 1,2,3-propanetriol in the liquid and 0.4 wt. % for 90 wt. % of 1,2,3-propanetriol in the liquid. The vapor-liquid equilibrium data of the ternary system are listed in Table IV and represented in Figure 2. All concentrations on the figure are expressed in mole fraction on 1,2,3-propanetriol–free basis, $X_A/(X_A + X_B)$ for the liquid phases, and similarly for the vapor phases, $Y_A/(Y_A + Y_B)$, the subscript A referring to 2-propanol and B to water. These values are also listed in Table IV.

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