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Molar heat capacities of some aqueous (2-amino-2-hydroxymethyl-1,3-propanediol + glycol) systems

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ABSTRACT

A new set of molar heat capacity data for aqueous {2-amino-2-hydroxymethyl-1,3-propanediol (TRIS) + glycol} at (30 to 80) °C and different concentrations (4% to 16% by weight TRIS or 56% to 44% by weight water, in a fixed amount of glycol – 40% by weight) were gathered via reliable measurement method and are presented in this report. The glycols considered were diethylene glycol (DEG), triethylene glycol (TEG), tetraethylene glycol (T_4EG), propylene glycol (PG), dipropylene glycol (DPG), and tripropylene glycol (TPG). The 198 data points gathered fit the equation, $C_p = C_{p,a} + B_1 m + B_2 m^2 + B_3 m^3$, where C_p and $C_{p,a}$ are the molar heat capacities of the (TRIS + glycol + water) and (water + glycol) systems, respectively, B_i the temperature-dependent parameters, and m the mole TRIS per kilogram (glycol + water). The overall average absolute deviation (AAD) of the experimental data from the corresponding values calculated from the correlation equation was 0.07%.

1. Introduction

The molecular structure of 2-amino-2-hydroxymethyl-1,3-propanediol (TRIS or THAM), a known biological buffer, suggests that it is a primary sterically-hindered alkanolamines; and, like most alkanolamines, TRIS, and other molecules of similar structures can be used for CO_2 absorption as some studies have already demonstrated [1,2]. Glycols, on the other hand, are known dehydrating agents. Mixing TRIS with glycol in water forms the so called glycol-amine solutions, which can be used to simultaneously absorb CO_2 and water, producing a high-purity treated gas [3]. Thus, the system (TRIS + glycol + water) can be a good alternative solvent for CO_2 from industrial effluent gases.

The enthalpy characteristics of the solvent system for CO_2 capture are important in the design of an effective equipment system for CO_2 capture, particularly in the energy-consuming solvent recovery phase. It was in this vein that we deemed it important to gather heat capacity data for this solvent system, which are indispensable in such process and equipment design. In this work, the representative systems are {TRIS + diethylene glycol (DEG) + H_2O}, {TRIS + triethylene glycol (TEG) + H_2O}, {TRIS + tetraethylene glycol (T_4EG) + H_2O}, {TRIS + propylene glycol (PEG) + H_2O}, {TRIS + dipropylene glycol (DPG) + H_2O}, and {TRIS + tripropylene glycol (TPG) + H_2O}. Molar heat capacities (for each system) at different component concentrations, *i.e.*, (4 to 16) wt.% TRIS or (56 to 44) wt.% H_2O, at fixed glycol concentration (40 wt.%), over the temperature range (30 to 80) °C, are reported in this paper.

2. Experimental

2.1. Chemicals

The specifications of chemicals used are listed in table 1. These chemical samples were used as received. The water used to prepare the aqueous solutions was Type I reagent grade (resistivity = 18.3 MΩ · cm; TOC < $15 \cdot 10^{-9}$), which was produced from our in-house compact deionizer (Barnstead Thermodyne Easy Pure 1052). A digital balance (Mettler-Toledo AL204) (accuracy = $\pm 1 \cdot 10^{-4}$ g) was used to weigh out the chemicals components of the solutions during preparation. The estimated uncertainty of the mole fraction of the aqueous solutions is $(1.5 \cdot 10^{-4}$. The solutions were degassed for up to 1.5 h using a vacuum pump (ULVAC SINKU KIKO GVD-050A) before measurement.

2.2. Property measurements

Prior to measurements involving the systems under study, measurement of molar heat capacity of water was performed to validate the procedures and equipment system used in this study.

The C_P values of the water and of the different TRIS/glycol/H_2O systems were measured using a differential scanning calorimeter (DSC) (DSC-2010) having a thermal analysis controller (TA Instruments). The DSC can operate from room temperature to 725 °C, with an uncertainty of ±0.1 K. Both the temperature and the heat

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TABLE 1
Specifications of chemicals samples.

Chemical name	Source	Mass fraction purity (as received)
Diethylene glycol (DEG)	TEDIA Co., Inc.	>0.999
Triethylene glycol (TEG)	TEDIA Co., Inc.	>0.9996
Tetraethylene glycol (T_4EG)	ACROS Organics	>0.995
Propylene glycol (PG)	ECHO Chemical Co., Ltd.	>0.998
Dipropylene glycol (DPG)	ACROS Organics	>0.99
Tripropylene glycol (TPG)	Alfa Aesar	>0.99
2-Amino-2-hydroxymethyl-1,3-propanediol (TRIS)	MP Biomedicals	>0.9995

TABLE 2
Heat capacity of DPG.

T/(°C)	Heat capacity C_P/(J · K^{-1} · mol^{-1})			
	Zaripov [5]	Union Carbide [7]	Li *et al.* [6]	This study
25.0	322.1			
26.7		326.9		
30.0			329.0	328.3 ± 1.6
37.8		333.7		
40.0			335.3	335.9 ± 1.5
48.9		340.4		
50.0			341.5	342.0 ± 1.3
60.0		347.2	348.8	348.5 ± 1.1
70.0			355.8	355.1 ± 0.8
71.1		354.5		
80.0			363.8	362.6 ± 0.1
% AAD[a]	0.88	0.36	0.13	0.14

$y_{calc.}$ is evaluated from equation (1).
y_{expt} refers to the experimental value in corresponding literature or study.
[a] % AAD $= \frac{100}{n}\sum_{i=1}^{n}\left|\frac{y_{expt}-y_{calc}}{y_{expt}}\right|_i$.

TABLE 3
Heat capacities and $(C_P - C_{P,a})$ of {TRIS (1) + DEG (2) + H_2O (3)}.

T/(°C)	Heat capacity C_P and $(C_P - C_{P,a})$/(J · K^{-1} · mol^{-1})					
	{TRIS (wt.%) + DEG (wt.%) + H_2O (wt.%)} molality, m_{TRIS}/(mol · kg^{-1})					
	(4/40/56) 0.34395		(9/40/51) 0.81642		(16/40/44) 1.57236	
	C_P	$C_P - C_{P,a}$	C_P	$C_P - C_{P,a}$	C_P	$C_P - C_{P,a}$
30.0	195.3	100.6	202.3	105.8	213.6	114.2
35.0	196.8	101.4	204.1	106.8	215.5	115.2
40.0	198.5	102.4	205.7	107.7	217.8	116.8
45.0	199.7	103.1	207.3	108.7	219.2	117.5
50.0	201.6	104.3	209.3	110.0	221.5	119.0
55.0	203.2	105.2	211.1	111.1	223.3	120.0
60.0	205.7	107.0	212.8	112.0	225.8	121.7
65.0	207.7	108.3	214.6	113.1	227.8	122.9
70.0	209.9	109.7	216.5	114.1	229.7	123.9
75.0	212.1	111.2	218.7	115.5	231.9	125.3
80.0	214.3	112.5	221.3	117.3	235.0	127.4

TABLE 4
Heat capacities and $(C_P - C_{P,a})$ of {TRIS (1) + TEG (2) + H_2O (3)}.

T/(°C)	Heat capacity C_P and $(C_P - C_{P,a})$/(J · K^{-1} · mol^{-1})					
	{TRIS (wt.%) + TEG (wt.%) + H_2O (wt.%)} molality, m_{TRIS}/(mol · kg^{-1})					
	(4/40/56) 0.34395		(9/40/51) 0.81642		(16/40/44) 1.57236	
	C_P	$C_P - C_{P,a}$	C_P	$C_P - C_{P,a}$	C_P	$C_P - C_{P,a}$
30.0	264.1	167.9	274.1	176.0	291.3	190.0
35.0	265.3	168.5	276.2	177.6	293.2	191.2
40.0	266.7	169.4	278.1	178.9	295.6	193.0
45.0	267.7	169.9	279.5	179.7	297.1	193.9
50.0	269.4	171.1	281.7	181.3	299.4	195.5
55.0	270.7	171.9	283.2	182.3	301.3	196.8
60.0	272.6	173.1	285.5	184.0	303.3	198.2
65.0	274.3	174.2	287.5	185.3	305.7	199.8
70.0	276.1	175.5	289.4	186.5	307.6	201.0
75.0	278.1	176.8	291.2	187.7	309.9	202.6
80.0	280.2	178.2	293.2	188.9	312.5	204.4