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Critical Point and Vapor Pressure Measurements for 17 Compounds by a Low Residence Time Flow Method[†]

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Critical temperature, critical pressure, and vapor pressure measurements have been performed on 15 compounds by a flow method with ultralow residence times. These compounds are γ-butyrolactone, di(propylene glycol), 1,3-butanediol, *N*-methyldiethanolamine, 4-formylmorpholine, 1,2-epoxy-2-methylpropane, diethyl oxalate, *n*-butyl acrylate, 2-(2-aminoethoxy)ethanol, *tert*-butyl acetate, 1,1-ethanediol diacetate, *p*-diisopropylbenzene, dimethyl disulfide, oxazole, and phenyl isocyanate. Accurate vapor pressure data are also included for di-*n*-butyl disulfide and sulfolane, but these compounds proved too unstable to directly determine the critical constants using this apparatus.

Introduction

This work is part of an ongoing investigation of the critical properties for compounds selected for industrial interest in 1999 and 2000 by sponsors of Project 851 of the Design Institute for Physical Properties (DIPPR) of the American Institute of Chemical Engineers (AIChE). This paper reports experimental measurements of the critical properties and vapor pressures for 15 compounds studied in a flow apparatus with ultralow residence times. These 15 compounds are as follows along with their Chemical Abstracts Registry Number (CASRN): γ-butyrolactone (96-48-0), di(propylene glycol) (25265-71-8), 1,3-butanediol (107-88-0), *N*-methyldiethanolamine (105-59-9), 4-formylmorpholine (4394-85-8), 1,2-epoxy-2-methylpropane (558-30-5), diethyl oxalate (95-92-1), *n*-butyl acrylate (141-32-2), 2-(2-aminoethoxy)ethanol (929-06-6), *tert*-butyl acetate (540-88-5), 1,1-ethanediol diacetate (542-10-9), *p*-diisopropylbenzene (100-18-5), dimethyl disulfide (624-92-0), oxazole (288-42-6), and phenyl isocyanate (103-71-9). Accurate vapor pressures are also reported for di-*n*-butyl disulfide (629-45-8) and sulfolane (126-33-0), but these compounds proved too unstable to determine the critical constants using this apparatus.

Experimental Section

The flow apparatus and procedures used for these measurements have been described previously.[1] In brief, the fluid to be tested flows at constant pressure through a capillary tube containing a thermocouple. As the temperature of the fluid increases, it goes through a phase change. Below the critical pressure, this material boils at "constant" temperature. Above the critical pressure, this change in state does not occur isothermally. This process produces temperature scans similar to the sample temperature scans for 2-(2-aminoethoxy)ethanol shown in Figure 1. This plot shows that, below the critical pressure, the temperature scan is flatter and shows a distinct break as the fluid goes from two phases to a single vapor phase. The scans above the critical point do not show this behavior. The reported critical point is between the lowest scan above the critical point and the highest scan below the critical point. Reported temperatures are based on the ITS-90. Temperature and pressure measurements have uncertainties of ± 0.1 K and ± 0.7 kPa, respectively.

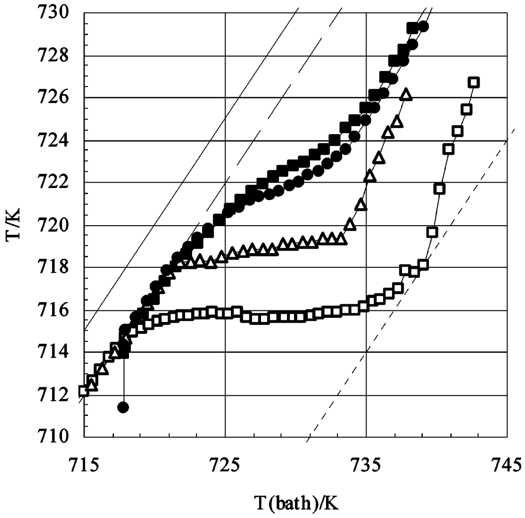

Figure 1. Sample temperature scans for 2-(2-aminoethoxy)ethanol. Temperature scans at □, 4521 kPa; △, 4729 kPa; ●, 4862 kPa; and ■, 4935 kPa. − −, no vaporization, - - -, full vaporization; —, $T = T$(bath).

Care was taken to purchase the compounds at high purity. Water and dissolved gases were removed by distilling off a small amount of material under vacuum, but no further attempts were made to purify the chemicals. Table 1 reports measured purities and water content for the compounds studied in this work. The purities were measured at Wiltec using gas chromatography. The water analyses were performed using Karl Fischer titration. These analyses were performed on the material after the distillation step. The supplier and CASRN of each chemical are also listed.

After flowing through the capillary where the vapor pressure and critical point measurements are made, the material collects in a receiving cylinder. For many of the compounds, samples were taken of the material in this receiving cylinder. These samples were then analyzed using gas chromatography to

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Table 1. Source and Purity of Materials

		mass fraction			
		analyzed purity			
compound	CASRN	Wiltec	supplier	water	supplier
γ-butyrolactone	96-48-0	0.997	0.994	0.0003	Aldrich
di(propylene glycol)[a]	25265-71-8	0.999+	0.9998	0.0003	DIPPR
1,3-butanediol	107-88-0	0.998	0.9974	0.00018	Aldrich
N-methyldiethanolamine	105-59-9	0.991	.0994	0.0006	Aldrich
4-formylmorpholine	4394-85-8	0.999	0.999	0.002	Aldrich
1,2-epoxy-2-methylpropane	558-30-5	0.997	0.99	0.0006	TCI
diethyl oxalate	95-92-1	0.997	0.999	0.0005	Aldrich
n-butyl acrylate	141-32-2	0.9996	0.999	0.0003	Aldrich
di-*n*-butyl disulfide	629-45-8	0.97	0.978	0.0001	DIPPR
2-(2-aminoethoxy)ethanol	929-06-6	0.997	0.990	0.0017	Aldrich
t-butyl acetate	540-88-5	0.999	0.999	0.0005	Aldrich
1,1-ethanediol diacetate	542-10-9	0.982	0.995	0.0001	Acros
p-diisopropyl benzene	100-18-5	0.999	0.997	0.00003	Acros
dimethyl disulfide	624-92-0	0.984	0.994	0.00002	Aldrich
oxazole	288-42-6	0.994	0.999	0.0038	DIPPR
phenyl isocyanate	103-71-9	0.996	0.994	0.00001	Acros
sulfolane	126-33-0	0.999+	0.999	0.0008	Aldrich

[a] Mixture of isomers.

Table 2. Critical Temperature T_c and Pressure p_c Measurements

Section A: Results of T_c and p_c Measurements on 15 Compounds

	T_c/K			p_c/MPa		
compound	measd[a]	previous	estd[b]	measd[a]	previous	estd[b]
γ-butyrolactone	732.5	731.0[c]	730	5.10	5.131[c]	7.02
di(propylene glycol)	705.2		698	3.38		3.43
1,3-butanediol	692.4	676.0[d]	703	5.18	4.02[d]	5.17
N-methyldiethanolamine	741.9		728	4.16		4.07
4-formylmorpholine	779.3		742	5.08		5.12
1,2-epoxy-2-methylpropane	499.9		509	4.35		5.12
diethyl oxalate	645.8	618.0[e]	604	3.06	2.14[e]	2.26
n-butyl acrylate	601.2		586	2.84		2.76
2-(2-aminoethoxy)-ethanol	721.2		705	4.80		4.65
tert-butyl acetate	541.2		526	3.04		2.87
1,1-ethanediol diacetate	618.2		601	2.97		2.99
p-diisopropyl benzene	676.2		680	2.36		2.31
dimethyl disulfide	607.8	615[f]	611	5.07		5.25
oxazole	550.8		541	6.77		7.06
phenyl isocyanate	656.9		649	4.00		4.07

Section B: Extrapolated T_c and p_c for Di-*n*-butyl Disulfide and Sulfolane

	T_c/K		p_c/MPa
compound	result[g]	estd[b]	estd[b]
di-*n*-butyl disulfide	711	716.3	2.47
sulfolane	868.2	837	6.06

[a] T_c and p_c for phenyl isocyanate have estimated uncertainties of ± 5 K and ± 5 %, respectively. Uncertainties for the other values are ± 2 K in T_c and ± 2 % in p_c. [b] Estimated critical temperatures based on the first order atomic contribution method of Wilson and Jasperson[2] using the boiling points measured as part of this project. Estimated critical pressures based on the estimated critical temperatures and the first order atomic contribution method of Wilson and Jasperson.[2] [c] Wilson et al.[3] report uncertainties of ± 0.2 K in T_c and ± 0.034 MPa in p_c. [d] Steele et al.[4] report uncertainties of ± 1 K in T_c and ± 0.2 MPa in p_c. [e] Steele et al.[5] do not report uncertainties for these values. [f] Anselme and Teja[6] report that, due to explosion, it can be concluded that the actual T_c is higher than this value. [g] p_c is estimated using the first-order atomic contribution method of Wilson and Jasperson[2] and the boiling points determined as part of this project. T_c is then obtained by extrapolating the vapor pressure equations reported in Tables 12 and 20 to these p_c values. p_c obtained in this fashion has an estimated uncertainty of ± 10 %, which translates into an uncertainty of ± 10 K in T_c.

determine how much the compound decomposed during the measurements. As suggested by the measured vapor pressures, both di-*n*-butyl disulfide and sulfolane showed significant decomposition, having purities less than 95 % after having flowed through the apparatus. In addition, 1,1-ethanediol diacetate also decomposed to where it had a purity less than 95 %. Because the residence time before the point where the measurements were made was less than 10 % of the residence time after this point, most of this decomposition would occur after the material has exited the capillary tubing where the measurements are made. The other analyzed compounds had purities better than 98 % after having flowed through the apparatus. Significant deviations from the “normal” shape of a vapor pressure curve are a good indication of when significant decomposition is occurring.

Results and Discussion

Table 2, Section A, presents the measured critical point values for 15 of the compounds included in this study as well as estimated critical point values for these compounds. The estimated critical temperatures were obtained using the boiling points reported in Table 3 and the first-order atomic contribution method of Wilson and Jasperson as presented in Poling et al.[2]

Table 3. Normal Boiling Points T_b Obtained from the Reported Correlations

	T_b/K	
compound	this work	previous
γ-butyrolactone	477.8	477.81^a
di(propylene glycol)	505.7	505.0^b
1,3-butanediol	481.4	481.38^c
N-methyldiethanolamine	520.7	
4-formylmorpholine	511.8	
1,2-epoxy-2-methylpropane	324.3	328.7^b
diethyl oxalate	458.5	458.611^d
n-butyl acrylate	419.7	419.771^e
di-*n*-butyl disulfide	509.1	
2-(2-aminoethoxy)ethanol	496.0	496.24^f
tert-butyl acetate	370.6	
1,1-ethanediol diacetate	439.5	
p-diisopropyl benzene	482.9	483.7^g
dimethyl disulfide	382.7	382.889^h
oxazole	342.7	
phenyl isocyanate	438.7	439.43^i
sulfolane	558.9	

[a] Ref 7. [b] Ref 8. [c] Ref 4. [d] Ref 5. [e] Ref 9. [f] Ref 10. [g] Ref 11. [h] Ref 12. [i] Ref 13.

Table 4. Vapor Pressure *p* of γ-Butyrolactone

T	*p*/kPa			*T*	*p*/kPa		
K	measd	corrld^a	% dev	K	measd	corrld^a	% dev
730.8	5013	5006	−0.13	477.81	101.3^b	101.3	−0.01
726.8	4779	4795	0.34	470.47	84.53^b	84.51	−0.03
713.8	4147	4161	0.33	463.16	70.12^b	70.08	−0.06
696.7	3454	3438	−0.44	455.88	57.82^b	57.76	−0.11
673.8	2643	2638	−0.18	448.64	47.38^b	47.31	−0.14
639.0	1723	1715	−0.46	441.43	38.57^b	38.49	−0.18
600.0	1005	1003	−0.12	434.29	31.18^b	31.14	−0.12
562.6	558.5	558.9	0.07	427.12	25.02^b	24.96	−0.25
532.5	325.8	326.9	0.34	420.02	19.93^b	19.88	−0.27
501.8	174.7	175.5	0.43	414.62	16.67^b	16.62	−0.27
474.90	93.29	94.35	1.14	408.11	13.33^b	13.29	−0.28
515.04	232.0^b	232.1	0.03	401.84	10.67^b	10.64	−0.25
507.52	198.5^b	198.5	0.02	394.08	7.999^b	7.984	−0.19
500.03	169.0^b	169.0	−0.01	383.72	5.333^b	5.330	−0.06
492.59	143.3^b	143.2	−0.01	367.39	2.666^b	2.673	0.26
485.19	120.8^b	120.8	0.01	361.09	2.000^b	2.010	0.50

[a] $A = 56.3367$, $B = -7691.91$, $C = -4.65838$, $D = 2.18881 \times 10^{-18}$. [b] Ref 7.

Table 5. Vapor Pressure *p* of Di(propylene glycol)

T	*p*/kPa			*T*	*p*/kPa		
K	measd	corrld^a	% dev	K	measd	corrld^a	% dev
703.4	3296	3292	−0.12	483.7	53.33^b	53.87	1.01
699.1	3123	3124	0.03	463.1	26.66^b	27.73	3.98
689.9	2779	2789	0.38	443.1	13.33^b	13.43	0.70
649.8	1631	1643	0.77	429.7	7.999^b	7.851	−1.86
607.2	854.3	860.1	0.69	420.6	5.333^b	5.314	−0.35
564.2	395.8	394.0	−0.45	404.5	2.666^c	2.518	−5.58
534.3	208.2	206.9	−0.62	389.4	1.333^c	1.161	−12.92
505.0	100.7	99.4	−1.30	375.3	0.667^c	0.524	−21.38
505.0	101.3^b	99.2	−2.08	347.0	0.133^c	0.083	−37.97

[a] $A = 112.270$, $B = -12847.2$, $C = -12.1096$, $D = 3.22954 \times 10^{-18}$. [b] Ref 8 used in correlation. [c] Ref 8 not used in correlation.

Table 6. Vapor Pressure *p* of 1,3-Butanediol

T	*p*/kPa			*T*	*p*/kPa		
K	measd	corrld^a	% dev	K	measd	corrld^a	% dev
688.2	4840	4867	0.55	457.269	47.38^b	47.34	−0.08
676.7	4158	4182	0.58	451.293	38.57^b	38.54	−0.06
662.5	3462	3453	−0.24	445.334	31.18^b	31.17	−0.03
646.7	2774	2772	−0.09	439.393	25.02^b	25.02	0.00
614.7	1719	1723	0.23	439.392	25.02^b	25.02	0.00
576.0	898.4	898.0	−0.04	433.47	19.93^b	19.94	0.05
537.8	418.5	420.4	0.45	428.953	16.67^b	16.68	0.07
508.1	209.6	209.4	−0.09	423.498	13.33^b	13.35	0.11
481.4	100.2	101.1	0.90	418.226	10.67^b	10.68	0.14
518.265	270.0^b	269.4	−0.23	411.676	7.999^b	8.014	0.18
512.054	232.0^b	231.5	−0.21	402.892	5.333^b	5.345	0.23
505.869	198.5^b	198.1	−0.20	396.948	4.000^b	4.010	0.24
499.706	169.0^b	168.7	−0.19	388.934	2.666^b	2.672	0.21
493.575	143.3^b	143.0	−0.18	384.978	2.183^b	2.169	−0.65
487.464	120.8^b	120.6	−0.17	383.502	2.000^b	2.003	0.17
481.38	101.3^b	101.2	−0.15	374.972	1.252^b	1.247	−0.40
475.319	84.53^b	84.41	−0.14	369.976	0.931^b	0.932	0.17
469.281	70.12^b	70.03	−0.12	364.978	0.690^b	0.690	−0.04
463.265	57.82^b	57.76	−0.10				

[a] $A = 119.350$, $B = -12930.4$, $C = -13.1187$, $D = 5.22941 \times 10^{-18}$. [b] Ref 4.

Table 7. Vapor Pressure *p* of *N*-Methyldiethanolamine

T	*p*/kPa			*T*	*p*/kPa		
K	measd	corrld^a	% dev	K	measd	corrld^a	% dev
738.4	3985	3968	−0.42	495.75	55.03^b	51.45	−6.51
735.4	3799	3833	0.89	490.85	48.25^b	44.57	−7.62
728.1	3475	3519	1.27	483.85	39.00^b	36.09	−7.45
707.5	2785	2742	−1.55	476.05	30.75^b	28.27	−8.08
657.1	1389	1395	0.42	467.85	23.43^b	21.63	−7.70
617.1	743.9	747.3	0.45	460.55	18.21^b	16.87	−7.36
574.8	346.1	344.3	−0.54	451.55	13.07^b	12.25	−6.22
543.3	175.1	175.2	0.04	443.35	9.439^b	9.030	−4.34
519.7	98.59	98.69	0.10	435.95	7.033^b	6.773	−3.70
513.85	90.44^b	84.85	−6.18	426.15	5.046^b	4.541	−10.01
506.55	74.75^b	69.72	−6.74	420.45	3.686^b	3.562	−3.38
501.35	64.45^b	60.35	−6.36				

[a] $A = 82.8943$, $B = -11011.8$, $C = -8.03383$, $D = 1.68146 \times 10^{-18}$. [b] Ref 14 not used in correlation. Daubert[15] later repeated measurements on this compound and reported results greater than 15 % higher than the correlation reported here.

Table 8. Vapor Pressure *p* of 4-Formylmorpholine

T	*p*/kPa			*T*	*p*/kPa		
K	measd	corrld^a	% dev	K	measd	corrld^a	% dev
777.7	4999	4956	−0.86	438.80	13.00^b	13.00	−0.01
775.2	4826	4825	−0.03	436.50	11.98^b	12.02	0.29
762.7	4137	4220	2.02	433.85	10.92^b	10.96	0.41
745.2	3447	3493	1.31	431.05	9.910^b	9.931	0.21
723.7	2761	2755	−0.22	429.45	9.480^b	9.380	−1.06
664.7	1382	1366	−1.16	425.95	8.440^b	8.264	−2.09
663.6	1379	1347	−2.29	419.15	6.490^b	6.413	−1.18
614.6	688.1	685.2	−0.42	416.45	5.800^b	5.783	−0.30
573.2	343.4	350.2	2.00	413.75	5.320^b	5.206	−2.15
538.0	174.8	179.5	2.69	411.85	4.810^b	4.830	0.41
507.5	91.70	91.60	−0.11	409.35	4.330^b	4.370	0.93
443.90	15.49^b	15.42	−0.45	406.30	3.830^b	3.861	0.81
442.90	15.00^b	14.92	−0.54	402.95	3.313^b	3.361	1.44
440.75	13.97^b	13.88	−0.58	400.85	3.018^b	3.076	1.93

[a] $A = 77.8856$, $B = -9819.26$, $C = -7.56946$, $D = 2.44682 \times 10^{-18}$. [b] Ref 16.

The estimated critical pressures were obtained using the estimated critical temperatures and the first-order atomic contribution method of Wilson and Jasperson.[2] Where available, measured values from the literature are also given. Due to plugging of the capillary tubing, fewer temperature scans for phenyl isocyanate were obtained in the critical region. On the basis of the difference between the highest scan below the critical point and the lowest scan above the critical point, the critical temperature and pressure reported in Table 2, Section A, for this compound have estimated uncertainties of ± 5 K and ± 5 %, respectively. The critical temperatures and pressures reported in Table 2, Section A, for the other compounds are estimated to have uncertainties of ± 2 K and ± 2 %, respectively. Due to the lower residence times possible with this method, these newly measured values are believed to be more reliable than the previous values reported in Table 2, Section A.

Sulfolane and di-*n*-butyl disulfide proved to be too unstable to directly measure the critical constants using this apparatus.

Table 9. Vapor Pressure p of 1,2-Epoxy-2-methylpropane

T	p/kPa			T	p/kPa		
K	measd	corrld[a]	% dev	K	measd	corrld[a]	% dev
499.2	4306	4308	0.03	309.2	53.33[b]	59.41	11.40
496.4	4141	4142	0.03	290.7	26.66[c]	28.50	6.88
469.4	2760	2778	0.65	274.4	13.33[c]	13.68	2.58
428.2	1381	1374	−0.52	263.5	7.999[c]	7.933	−0.83
393.2	678.4	671.1	−1.08	255.9	5.333[c]	5.271	−1.16
365.6	348.9	344.6	−1.21	243.7	2.666[c]	2.585	−3.04
339.1	165.1	163.1	−1.23	232.9	1.333[c]	1.289	−3.33
320.1	87.08	87.96	1.01	223.2	0.667[c]	0.649	−2.59
328.7	101.3[b]	117.2	15.70	204.2	0.133[c]	0.139	4.34

[a] $A = 32.7606$, $B = -4019.925$, $C = -1.52940$, $D = 4.53506 \times 10^{-18}$. [b] Ref 8 not used in correlation. [c] Ref 8 used in correlation.

Table 10. Vapor Pressure p of Diethyl Oxalate

T	p/kPa			T	p/kPa		
K	measd	corrld[a]	% dev	K	measd	corrld[a]	% dev
644.4	3013	3004	−0.29	445.318	70.12[b]	70.19	0.10
642.5	2934	2927	−0.24	438.730	57.82[b]	57.85	0.05
638.8	2761	2781	0.74	432.182	47.38[b]	47.37	0.00
590.1	1381	1378	−0.22	425.673	38.57[b]	38.54	−0.06
547.3	690.9	686.4	−0.65	419.203	31.18[b]	31.14	−0.11
512.9	359.9	358.9	−0.29	412.772	25.02[b]	24.98	−0.15
481.8	182.4	181.6	−0.41	412.770	25.02[b]	24.98	−0.16
454.6	90.67	90.96	0.32	406.380	19.93[b]	19.89	−0.19
499.404	270.0[b]	270.7	0.27	401.523	16.67[b]	16.63	−0.21
492.514	232.0[b]	232.6	0.27	395.674	13.33[b]	13.30	−0.23
485.663	198.5[b]	199.0	0.28	390.042	10.67[b]	10.64	−0.22
478.844	169.0[b]	169.5	0.27	383.073	7.999[b]	7.983	−0.20
472.061	143.3[b]	143.6	0.24	373.779	5.333[b]	5.327	−0.11
465.315	120.8[b]	121.1	0.22	367.529	4.000[b]	4.000	0.01
458.611	101.3[b]	101.5	0.19	359.151	2.666[b]	2.672	0.21
451.946	84.53[b]	84.66	0.15	353.500	2.000[b]	2.008	0.38

[a] $A = 89.3688$, $B = -9689.53$, $C = -9.26533$, $D = 7.19290 \times 10^{-18}$. [b] Ref 5.

Table 11. Vapor Pressure p of *n*-Butyl Acrylate

T	p/kPa			T	p/kPa		
K	measd	corrld[a]	% dev	K	measd	corrld[a]	% dev
599.1	2761	2768	0.26	375.405	25.02[b]	24.98	−0.17
549.3	1380	1374	−0.45	375.403	25.02[b]	24.98	−0.18
506.5	689.5	684.8	−0.67	369.243	19.93[b]	19.89	−0.22
471.9	351.6	353.0	0.39	364.565	16.67[b]	16.62	−0.24
441.9	178.6	179.9	0.75	358.938	13.33[b]	13.30	−0.26
419.771	101.3[b]	101.6	0.27	353.523	10.67[b]	10.64	−0.25
413.303	84.53[b]	84.72	0.23	346.831	7.999[b]	7.981	−0.22
406.878	70.12[b]	70.24	0.17	337.919	5.333[b]	5.327	−0.10
400.495	57.82[b]	57.88	0.10	331.929	4.000[b]	4.000	0.01
394.157	47.38[b]	47.39	0.03	323.914	2.666[b]	2.673	0.25
387.862	38.57[b]	38.55	−0.04	318.513	2.000[b]	2.009	0.43
381.611	31.18[b]	31.14	−0.11				

[a] $A = 72.0384$, $B = -7685.19$, $C = -6.99431$, $D = 7.68638 \times 10^{-18}$. [b] Ref 9.

Table 12. Vapor Pressure p of Di-*n*-Butyl Disulfide

T	p/kPa			T	p/kPa		
K	measd	corrld[a]	% dev	K	measd	corrld[a]	% dev
695.2	2413[b]	2025	−16.08	571.7	349.6	351.1	0.44
689.5	2069[b]	1885	−8.89	535.7	180.3	179.6	−0.39
659.9	1377[b]	1291	−6.25	504.2	90.32	90.03	−0.33
614.9	695.7	694.9	−0.11				

[a] $A = 110.4949$, $B = -11890.8$, $C = -12.1477$, $D = 5.55799 \times 10^{-18}$. [b] Measured points not used in correlation due to decomposition.

Table 13. Vapor Pressure p of 2-(2-Aminoethoxy)ethanol

T	p/kPa			T	p/kPa		
K	measd	corrld[a]	% dev	K	measd	corrld[a]	% dev
719.4	4729	4702	−0.58	476.64	57.82[b]	57.96	0.25
716.5	4521	4548	0.59	470.16	47.38[b]	47.45	0.15
685.0	3130	3124	−0.19	463.71	38.57[b]	38.60	0.08
653.9	2085	2087	0.12	457.28	31.18[b]	31.18	0.00
625.9	1395	1399	0.29	450.87	25.02[b]	25.00	−0.08
594.2	842.6	843.6	0.11	444.49	19.93[b]	19.91	−0.12
564.9	496.6	495.2	−0.29	439.63	16.67[b]	16.64	−0.15
526.9	225.2	220.8	−1.93	433.76	13.33[b]	13.31	−0.19
500.9	117.3	115.6	−1.40	428.1	10.67[b]	10.65	−0.18
516.09	169.0[b]	170.4	0.82	421.07	7.999[b]	7.985	−0.17
509.45	143.3[b]	144.3	0.74	411.66	5.333[b]	5.327	−0.11
502.82	120.8[b]	121.5	0.62	405.31	4.000[b]	3.999	−0.02
496.24	101.3[b]	101.9	0.54	396.76	2.666[b]	2.669	0.11
489.68	84.53[b]	84.91	0.45	390.97	2.000[b]	2.004	0.20
483.15	70.12[b]	70.37	0.36				

[a] $A = 99.0087$, $B = -11709.0$, $C = -10.2984$, $D = 2.72475 \times 10^{-18}$. [b] Ref 10.

Table 14. Vapor Pressure p of *tert*-Butyl Acetate

T	p/kPa			T	p/kPa		
K	measd	corrld[a]	% dev	K	measd	corrld[a]	% dev
538.6	2949	2929	0.66	394.95	213.7[b]	202.4	5.28
537.7	2903	2893	0.34	389.05	233.5[b]	172.9	25.94
537.3	2868	2875	−0.23	384.55	158.6[b]	152.7	3.70
536.4	2835	2838	−0.09	381.85	149.3[b]	141.5	5.24
535.9	2801	2819	−0.63	376.65	120.4[b]	121.7	−1.07
535.7	2802	2812	−0.36	373.55	111.4[b]	111.0	0.41
533.7	2722	2731	−0.30	368.85	105.8[b]	96.1	9.20
514.5	2074	2059	0.73	368.45	94.11[c]	94.91	−0.85
495.0	1527	1524	0.21	365.55	86.21[c]	86.63	−0.49
472.7	1053	1052	0.09	362.35	77.92[c]	78.17	−0.32
518.85	5215[b]	2197	57.87	357.85	67.15[c]	67.38	−0.34
507.05	4358[b]	1838	57.82	353.25	57.55[c]	57.60	−0.09
495.25	3452[b]	1529	55.72	349.35	50.36[c]	50.23	0.26
484.95	2616[b]	1293	50.56	344.35	41.99[c]	41.90	0.21
469.15	1676[b]	988	41.04	339.05	34.29[c]	34.32	−0.10
455.35	1299[b]	769	40.81	332.25	26.32[c]	26.26	0.21
438.15	855.0[b]	549.3	35.75	326.45	20.88[c]	20.67	0.98
425.05	480.5[b]	416.3	13.35	320.25	15.80[c]	15.82	−0.12
415.25	376.7[b]	333.8	11.38	314.25	12.25[c]	12.05	1.62
408.65	397.1[b]	285.6	28.08	309.05	9.553[c]	9.425	1.34
403.55	290.3[b]	252.1	13.16	305.45	7.899[c]	7.901	−0.02
399.65	320.7[b]	228.5	28.74	301.35	6.253[c]	6.422	−2.70

[a] $A = 74.7030$, $B = -6914.69$, $C = -7.53331$, $D = 16.5062 \times 10^{-18}$. [b] Ref 17 high-pressure data not used in correlation. [c] Ref 17 low-pressure data used in correlation.

Table 2, Section B, presents estimated critical properties for these compounds. The critical pressure is estimated using the normal boiling point reported in Table 3 and the first-order method of Wilson and Jasperson.[2] The reported critical temperature is then obtained by extrapolating the vapor pressure equation obtained as part of this project to this estimated critical pressure. It is estimated that the critical pressure obtained in this fashion is uncertain to within ± 10 %, which translates into an uncertainty of ± 10 K in the critical temperature. The authors feel that this is better than extrapolating to an estimated critical temperature because the normal uncertainty associated with an estimated critical temperature would translate into a large uncertainty in the extrapolated critical pressure.

Table 3 presents the normal boiling point for each of the compounds included in this study. The values from this work were obtained using the reported correlations given at the bottom of Tables 4 through 20. Measured boiling points reported by other researchers listed in Tables 4 through 20 are also listed. Note that the data measured as part of this work for *tert*-butyl acetate, dimethyl disulfide, and oxazole do not extend down to near the boiling point. For these compounds, the reported T_b depends strongly on the literature vapor pressures used in the correlation. For the remainder of the compounds, the data measured for this works extends down to 280 kPa or less. For about half of the compounds, the data measured as part of this project extend down below the normal boiling point.

Tables 4 through 20 present vapor pressure data on the 17 compounds included in this study. These tables list the measured

Table 15. Vapor Pressure *p* of 1,1-Ethanediol Diacetate

T	*p*/kPa			*T*	*p*/kPa		
K	measd	corrld[a]	% dev	K	measd	corrld[a]	% dev
612.0	2697	2706	−0.32	423.15	62.93[b]	62.61	0.50
608.2	2561	2555	0.23	413.15	45.33[b]	45.38	−0.11
601.1	2286	2293	−0.30	403.15	32.40[b]	32.15	0.75
571.5	1457	1455	0.12	393.15	22.67[b]	22.22	1.96
541.2	902.2	891.7	1.16	383.15	15.07[b]	14.94	0.81
514.2	555.5	552.7	0.50	373.15	9.866[b]	9.752	1.16
486.4	314.3	318.4	−1.32	363.15	6.000[b]	6.158	−2.63
461.6	177.6	180.9	−1.84	353.15	3.600[b]	3.750	−4.17
433.15	84.66[b]	84.61	0.06	343.15	2.267[b]	2.194	3.19

[a] $A = 126.696$, $B = -11527.4$, $C = -14.6340$, $D = 16.2526 \times 10^{-18}$.
[b] Ref 18.

Table 16. Vapor Pressure *p* of *p*-Diisopropylbenzene

T	*p*/kPa			*T*	*p*/kPa		
K	measd	corrld[a]	% dev	K	measd	corrld[a]	% dev
675.9	2325	2342	0.71	412.8	13.33[b]	13.24	−0.73
672.3	2258	2242	−0.69	407.1	10.67[b]	10.79	1.19
666.2	2078	2084	0.30	399.2	7.999[b]	8.039	0.50
648.1	1669	1669	−0.02	394.4	6.666[b]	6.674	0.12
648.1	1667	1669	0.08	388.8	5.333[b]	5.334	0.02
596.8	837.8	836.2	−0.19	382.2	4.000[b]	4.054	1.35
552.6	416.3	416.3	−0.01	372.8	2.666[b]	2.686	0.75
518.0	217.1	218.3	0.55	366.6	2.000[b]	2.019	0.98
483.7	101.3[b]	103.2	1.82	358.2	1.333[b]	1.346	0.97
480.2	93.33[b]	94.86	1.64	353.5	1.067[b]	1.062	−0.44
473.2	79.99[b]	79.83	−0.21	348.1	0.800[b]	0.801	0.14
465.8	66.66[b]	66.05	−0.91	344.6	0.667[b]	0.664	−0.46
457.5	53.33[b]	52.93	−0.75	340.7	0.533[b]	0.535	0.32
446.9	40.00[b]	39.30	−1.75	335.4	0.400[b]	0.395	−1.12
433.2	26.66[b]	26.03	−2.37	328.7	0.267[b]	0.265	−0.43
424.7	20.00[b]	19.83	−0.84				

[a] $A = 75.8188$, $B = -9000.99$, $C = -7.39501$, $D = 3.68052 \times 10^{-18}$.
[b] Ref 11.

Table 17. Vapor Pressure *p* of Dimethyl Disulfide

T	*p*/kPa			*T*	*p*/kPa		
K	measd	corrld[a]	% dev	K	measd	corrld[a]	% dev
607.2	5037	5048	−0.22	352.351	38.55[b]	38.50	0.13
604.8	4902	4909	−0.16	346.384	31.16[b]	31.09	0.21
591.4	4205	4197	0.21	340.451	25.01[b]	24.93	0.32
561.0	2897	2888	0.33	334.561	19.92[b]	19.83	0.43
533.1	2002	1992	0.50	333	18.80[b]	18.75	0.27
500.8	1244	1238	0.50	328	15.36[b]	15.30	0.37
466.3	690.0	690.4	−0.06	323	12.44[b]	12.39	0.42
401.761	169.1[b]	170.4	−0.77	318	9.999[b]	9.958	0.41
395.423	143.3[b]	144.2	−0.67	313	7.970[b]	7.939	0.39
389.134	120.8[b]	121.5	−0.57	308	6.293[b]	6.275	0.28
382.889	101.3[b]	101.8	−0.46	303	4.924[b]	4.916	0.15
376.690	84.53[b]	84.82	−0.34	298	3.818[b]	3.815	0.08
370.543	70.11[b]	70.28	−0.24	293	2.930[b]	2.932	−0.04
364.433	57.80[b]	57.87	−0.11	288	2.226[b]	2.229	−0.12
358.368	47.36[b]	47.35	0.01	273.15	0.905[b]	0.915	−1.03

[a] $A = 55.1889$, $B = -5991.31$, $C = -4.71281$, $D = 6.32551 \times 10^{-18}$.
[b] Ref 12. Ref 19 also measured data on this compound over a smaller range. These data agreed very well with the data of Scott et al.[12]

temperature and the measured and correlated vapor pressures. The reported correlations of the measured data demonstrate the internal consistency of the measured data and show, where applicable, that these data agree with data previously measured on these compounds. The Riedel equation[2] was used to correlate the data in this study and is given below:

$$\ln(p/\mathrm{Pa}) = A + \frac{B}{T/\mathrm{K}} + C \ln(T/\mathrm{K}) + D(T/\mathrm{K})^6$$

where A, B, C, and D are parameters. The values for these parameters obtained from a least-squares regression are given at the bottom of each table. The vapor pressures measured as part of this project have an estimated uncertainty of ± 2 %.

Table 18. Vapor Pressure *p* of Oxazole

T	*p*/kPa			*T*	*p*/kPa		
K	measd	corrld[a]	% dev	K	measd	corrld[a]	% dev
547.4	6492	6474	0.28	335.92	79.99[b]	80.03	−0.05
535.5	5523	5536	−0.23	330.89	66.66[b]	66.65	0.02
514.9	4146	4169	−0.54	324.97	53.33[b]	53.28	0.09
494.6	3116	3097	0.61	317.7	40.00[b]	39.94	0.13
479.0	2424	2426	−0.08	308.08	26.66[b]	26.62	0.15
344.23	106.7[b]	106.8	−0.15	293.16	13.33[b]	13.35	−0.14
340.31	93.33[b]	93.41	−0.09				

[a] $A = 54.0394$, $B = -5525.14$, $C = -4.52398$, $D = 9.75862 \times 10^{-18}$.
[b] Ref 20.

Table 19. Vapor Pressure *p* of Phenyl Isocyanate

T	*p*/kPa			*T*	*p*/kPa		
K	measd	corrld[a]	% dev	K	measd	corrld[a]	% dev
653.1	3793	3807	−0.36	405.01	38.57[b]	38.63	−0.16
653.0	3795	3802	−0.18	398.25	31.18[b]	31.14	0.10
618.6	2551	2563	−0.46	391.52	25.02[b]	24.93	0.35
588.3	1724	1733	−0.54	384.84	19.93[b]	19.83	0.52
553.2	1038	1036	0.12	379.76	16.67[b]	16.56	0.63
479.7	278.9	268.4	3.76	373.65	13.33[b]	13.24	0.69
445.48	120.8[b]	120.8	0.02	367.77	10.67[b]	10.59	0.67
439.43	101.3[b]	103.3	−2.00	360.49	7.999[b]	7.951	0.60
432.47	84.54[b]	85.88	−1.59	350.78	5.333[b]	5.315	0.35
425.54	70.12[b]	70.95	−1.18	344.26	4.000[b]	3.999	0.02
418.65	57.82[b]	58.27	−0.79	329.64	2.000[b]	2.023	−1.13
411.81	47.38[b]	47.59	−0.46				

[a] $A = 40.2744$, $B = -6111.43$, $C = -2.43583$, $D = 0.313416 \times 10^{-18}$.
[b] Ref 13.

Table 20. Vapor Pressure *p* of Sulfolane

T	*p*/kPa			*T*	*p*/kPa		
K	measd	corrld[a]	% dev	K	measd	corrld[a]	% dev
848.2	5861[b]	5001	14.68	542.06	70.13[c]	70.33	−0.28
845.9	5523[b]	4891	11.45	533.62	57.82[c]	57.94	−0.22
840.0	5173[b]	4619	10.72	525.22	47.37[c]	47.44	−0.14
836.9	4833[b]	4479	7.32	516.89	38.59[c]	38.61	−0.06
834.6	4493[b]	4380	2.52	508.56	31.18[c]	31.18	0.00
829.0	4144	4146	−0.05	500.29	25.02[c]	25.01	0.05
802.7	3185	3189	−0.15	500.29	25.03[c]	25.01	0.07
773.4	2363	2353	0.43	492.06	19.93[c]	19.91	0.09
742.0	1665	1666	−0.09	485.80	16.66[c]	16.64	0.14
713.2	1181	1186	−0.37	478.25	13.32[c]	13.30	0.14
685.1	829.2	828.2	0.13	470.98	10.66[c]	10.64	0.19
656.3	556.8	555.2	0.29	462.04	8.007[c]	7.992	0.18
626.3	350.2	350.7	−0.15	449.99	5.331[c]	5.323	0.14
594.4	203.9	202.9	0.49	441.88	3.993[c]	3.991	0.03
560.2	103.6	104.1	−0.47	423.82	2.000[c]	2.008	−0.37

[a] $A = 61.4707$, $B = -9377.91$, $C = -5.24771$, $D = 1.06419 \times 10^{-18}$.
[b] Measured vapor pressure not used in correlation due to decomposition.
[c] Ref 21.

For di(propylene glycol) (Table 5) and 1,2-epoxy-2-methylpropane (Table 9), several of the points reported by Stull[8] are not used in obtaining the reported correlation. These points do not agree with the rest of the reported data. In the case of *N*-methyldiethanolamine, the correlation reported at the bottom of Table 7 is based solely on the data measured as part of this project. This table shows that the data reported by Daubert and Hutchison[14] are about 10 % higher than extrapolated values obtained from this correlation. A few years later, Daubert[15] repeated measurements on this compound and reported different results. Data from this latter set of measurements are not shown in Table 7 because they are greater than 15 % higher than the correlation reported here. For *tert*-butyl acetate (Table 14), the "high-pressure data" reported by Daubert[17] are not used in obtaining the reported correlation.

Because of decomposition, some of the measured vapor pressures for di-*n*-butyl disulfide (Table 12) and sulfolane (Table

20) are not used in correlating the measured data. Stull[8] reports data for di-*n*-butyl disulfide, but his data include a normal boiling point nearly 100 K higher than the normal boiling point obtained for this project. Because his data are so different from the data reported here, they have been left out. White et al.[19] report attempting vapor pressure measurements on this compound but were unable to obtain consistent results.

Because there are only four good vapor pressure points for di-*n*-butyl disulfide, a few values are estimated down to about 12 kPa. White et al.[19] showed that, at a given pressure, the boiling points of dimethyl disulfide, diethyl disulfide, and dipropyl disulfide are approximately a linear function of chain length. Using data for these three compounds, boiling points for di-*n*-butyl disulfide at three pressures from (12 to 50) kPa are estimated and used in obtaining the parameters at the bottom of Table 12.

Conclusion

Accurate vapor pressures have been measured on 17 compounds of industrial significance, and reliable critical point values have been measured for 15 of these 17 compounds. The critical point values of di-*n*-butyl disulfide and sulfolane were not obtained using this apparatus because these compounds proved too unstable. Using the measured vapor pressure data, reasonable estimates for the critical temperature and pressure of these two compounds were obtained and reported. These data are useful in many engineering applications and in evaluating the applicability of current predictive techniques. They will also be useful in developing better correlations for estimating critical temperatures and pressures.

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