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THERMODYNAMIC FUNCTIONS OF NAPHTHALENE FROM 0.25 TO 8 ATM

F. BENNETT, Jr. *, D.G. McFEE and J. LIELMEZS

Department of Chemical Engineering, The University of British Columbia, Vancouver, B.C. (Canada)

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ABSTRACT

Real gas thermodynamic functions, C_p, S, $(H-H_0)/T$, and $-(F-H_0)/T$, have been calculated for naphthalene from 0.25 to 8 atm within the temperature range 273.15–1200 K, correcting the thermodynamic property ideal gas values by means of the Berthelot equation of state.

INTRODUCTION

In this work, using the ideal gas state thermodynamic property values of naphthalene as obtained by Lielmezs et al. [1] and correcting these values by means of the Berthelot equation of state, temperature- and pressure-dependent thermodynamic functions C_p, S, $(H-H_0)/T$ and $-(F-H_0)/T$ have been calculated from 0.25 to 8 atm within the temperature range 273.15–1200 K (Table 1).

The calculated thermodynamic function values for both of the proposed sets of assignments (A and B, see ref. 1) have been correlated by a five constant polynomial

$$\Lambda = a + bT + cT^2 + dT^3 + eT^4 \tag{1}$$

where Λ is the real gas thermodynamic function at temperature T and pressure P. The constants a, b, c, d and e [eqn. (1)] were obtained using linear least squares curve fitting methods [2] and are found in Table 2. All of the assigned frequencies (both sets, A and B) as well as other values of molecular parameters used ** are found in the work of Lielmezs et al. [1].

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* Present address: Texaco Canada Resources Ltd., Willesdan Green, Alta., Canada.

** The values of critical parameters used have been taken from ref. 4: critical temperature, $T_c = 748.4$ K: critical pressure, $P_c = 40.0$ atm.

TABLE I

Heat capacity, enthalpy and free energy functions and entropy for assignment sets A and B

Temp. (K)	C_p (cal g^{-1} mole^{-1} K^{-1})		$(H-H_0)/T$ (cal g^{-1} mole^{-1} K^{-1})		$-(F-H_0)/T$ (cal g^{-1} mole^{-1} K^{-1})		S (cal g^{-1} mole^{-1} K^{-1})	
	A	B	A	B	A	B	A	B
$P=0.25$ atm								
451.00	48.67	48.39	24.68	24.52	74.12	74.04	98.81	98.56
522.70	54.86	54.61	28.41	28.23	78.04	77.93	106.44	106.16
273.15	29.53	29.27	15.07	15.00	64.36	64.34	79.43	79.33
298.15	32.40	32.11	16.40	16.31	65.74	65.71	82.14	82.02
300.00	32.61	32.33	16.50	16.41	65.84	65.81	82.34	82.22
350.00	38.29	37.99	19.21	19.09	68.59	68.54	87.80	87.63
400.00	43.66	43.36	21.94	21.79	71.33	71.26	93.27	93.06
450.00	48.58	48.29	24.63	24.47	74.07	73.99	98.70	98.45
500.00	53.00	52.74	27.25	27.08	76.80	76.70	104.05	103.78
550.00	56.97	56.73	29.77	29.59	79.52	79.40	109.29	108.99
600.00	60.51	60.29	32.19	32.01	82.21	82.08	114.40	114.08
650.00	63.69	63.49	34.49	34.31	84.88	84.73	119.37	119.04
700.00	66.54	66.36	36.68	36.50	87.52	87.35	124.20	123.85
750.00	69.12	68.95	38.76	38.57	90.12	89.94	128.88	128.52
800.00	71.45	71.30	40.73	40.55	92.68	92.50	133.41	133.05
850.00	73.57	73.44	42.60	42.42	95.21	95.01	137.81	137.43
900.00	75.51	75.39	44.38	44.20	97.69	97.49	142.07	141.69
950.00	77.28	77.17	46.06	45.89	100.14	99.92	146.20	145.81
1000.00	78.91	78.80	47.67	47.49	102.54	102.32	150.21	149.81
1050.00	80.40	80.31	49.19	49.02	104.91	104.67	154.10	153.69
1100.00	81.77	81.69	50.64	50.47	107.23	106.99	157.87	157.46
1150.00	83.04	82.96	52.02	51.86	109.51	109.26	161.53	161.12
1200.00	84.21	84.13	53.34	53.18	111.75	111.50	165.09	164.68
$P=0.50$ atm								
451.00	48.81	48.53	24.61	24.45	72.77	72.69	97.38	97.14
522.70	54.95	54.70	28.36	28.19	76.67	76.56	105.03	104.75
273.15	30.17	29.91	14.75	14.67	63.09	63.07	77.84	77.74
298.15	32.89	32.61	16.16	16.06	64.44	64.41	80.60	80.48
300.00	33.10	32.81	16.26	16.17	64.54	64.51	80.80	80.68
350.00	38.60	38.30	19.06	18.94	67.26	67.21	86.32	86.15
400.00	43.87	43.57	21.84	21.69	69.98	69.92	91.82	91.61
450.00	48.72	48.44	24.56	24.40	72.71	72.63	97.27	97.03
500.00	53.11	52.85	27.20	27.02	75.44	75.34	102.64	102.36
550.00	57.05	56.81	29.74	29.56	78.15	78.03	107.89	107.59
600.00	60.57	60.35	32.16	31.98	80.84	80.71	113.00	112.69
650.00	63.73	63.54	34.47	34.28	83.51	83.36	117.98	117.65
700.00	66.58	66.40	36.66	36.48	86.14	85.98	122.81	122.46

Table 1 (continued)

Temp. (K)	C_p (cal g^{-1} mole^{-1} K^{-1})		$(H-H_0)/T$ (cal g^{-1} mole^{-1} K^{-1})		$-(F-H_0)/T$ (cal g^{-1} mole^{-1} K^{-1})		S (cal g^{-1} mole^{-1} K^{-1})	
	A	B	A	B	A	B	A	B
750.00	69.15	68.98	38.75	38.56	88.75	88.57	127.49	127.13
800.00	71.48	71.33	40.72	40.54	91.31	91.12	132.03	131.66
850.00	73.60	73.46	42.59	42.41	93.83	93.64	136.43	136.05
900.00	75.53	75.41	44.37	44.19	96.32	96.11	140.69	140.30
950.00	77.30	77.19	46.06	45.88	98.76	98.55	144.82	144.43
1000.00	78.92	78.82	47.66	47.49	101.17	100.94	148.83	148.43
1050.00	80.41	80.32	49.18	49.02	103.53	103.30	152.71	152.31
1100.00	81.78	81.70	50.64	50.47	105.85	105.61	156.49	156.08
1150.00	83.05	82.97	52.02	51.86	108.13	107.88	160.15	159.74
1200.00	84.21	84.14	53.33	53.18	110.38	110.12	163.71	163.30
$P=1.0$ atm								
451.00	49.10	48.82	24.47	24.31	71.44	71.35	95.91	95.66
522.70	55.14	54.88	28.27	28.10	75.32	75.21	103.60	103.31
273.15	31.47	31.21	14.11	14.03	61.92	61.90	76.03	75.93
298.15	33.89	33.61	15.67	15.57	63.22	63.19	78.89	78.77
300.00	34.07	33.79	15.78	15.68	63.32	63.29	79.10	78.98
350.00	39.21	38.91	18.76	18.63	65.98	65.93	84.74	84.57
400.00	44.28	43.98	21.63	21.49	68.67	68.61	90.31	90.10
450.00	49.01	48.73	24.42	24.25	71.38	71.30	95.80	95.55
500.00	53.32	53.06	27.09	26.92	74.09	73.99	101.19	100.92
550.00	57.20	56.96	29.66	29.48	76.80	76.68	106.46	106.16
600.00	60.69	60.48	32.10	31.92	79.48	79.35	111.59	111.27
650.00	63.83	63.63	34.42	34.24	82.15	82.00	116.57	116.24
700.00	66.65	66.48	36.63	36.44	84.78	84.62	121.40	121.06
750.00	69.21	69.05	38.72	38.53	87.38	87.20	126.09	125.73
800.00	71.53	71.38	40.70	40.51	89.94	89.75	130.63	130.26
850.00	73.64	73.50	42.57	42.39	92.46	92.27	135.03	134.66
900.00	75.57	75.44	44.35	44.17	94.95	94.74	139.30	138.91
950.00	77.33	77.22	46.04	45.87	97.39	97.17	143.43	143.04
1000.00	78.95	78.84	47.65	47.48	99.79	99.57	147.44	147.04
1050.00	80.43	80.34	49.17	49.01	102.16	101.92	151.33	150.93
1100.00	81.80	81.72	50.63	50.46	104.48	104.23	155.10	154.70
1150.00	83.07	82.98	52.01	51.85	106.76	106.51	158.77	158.36
1200.00	84.23	84.15	53.33	53.17	109.00	108.74	162.33	161.91
$P=2.0$ atm								
451.00	49.67	49.39	24.19	24.03	70.15	70.07	94.34	94.09
522.70	55.50	55.25	28.09	27.92	74.00	73.89	102.10	101.81
273.15	34.05	33.79	12.83	12.75	60.96	60.94	73.79	73.69
298.15	35.88	35.59	14.68	14.59	62.17	62.14	76.85	76.73

Table 1 (continued)

Temp. (K)	C_p (cal g^{-1} mole^{-1} K^{-1})		$(H-H_0)/T$ (cal g^{-1} mole^{-1} K^{-1})		$-(F-H_0)/T$ (cal g^{-1} mole^{-1} K^{-1})		S (cal g^{-1} mole^{-1} K^{-1})	
	A	B	A	B	A	B	A	B
300.00	36.02	35.74	14.81	14.72	62.26	62.23	77.07	76.95
350.00	40.44	40.14	18.15	18.03	64.80	64.75	82.95	82.78
400.00	45.10	44.80	21.23	21.08	67.43	67.36	88.65	88.44
450.00	49.59	49.30	24.13	23.97	70.10	70.01	94.23	93.98
500.00	53.74	53.48	26.89	26.72	72.78	72.68	99.67	99.40
550.00	57.52	57.28	29.50	29.33	75.47	75.35	104.97	104.68
600.00	60.94	60.72	31.98	31.80	78.14	78.01	110.13	109.81
650.00	64.02	63.82	34.33	34.15	80.80	80.65	115.13	114.79
700.00	66.81	66.63	36.55	36.37	83.42	83.26	119.98	119.63
750.00	69.33	69.17	38.66	38.47	86.02	85.84	124.67	124.31
800.00	71.63	71.48	40.65	40.46	88.58	88.39	129.22	128.85
850.00	73.72	73.59	42.53	42.35	91.10	90.90	133.63	133.25
900.00	75.64	75.51	44.32	44.14	93.58	93.37	137.90	137.51
950.00	77.39	77.28	46.01	45.84	96.02	95.80	142.03	141.64
1000.00	79.00	78.90	47.62	47.45	98.42	98.20	146.05	145.65
1050.00	80.48	80.38	49.15	48.99	100.78	100.55	149.94	149.53
1100.00	81.84	81.75	50.61	50.44	103.10	102.86	153.71	153.31
1150.00	83.10	83.02	51.99	51.83	105.38	105.14	157.38	156.97
1200.00	84.26	84.18	53.32	53.16	107.63	107.37	160.94	160.53
$P=4.0$ atm								
451.00	50.82	50.54	23.63	23.46	68.95	68.87	92.58	92.33
522.70	56.24	55.99	27.73	27.56	72.74	72.63	100.47	100.19
273.15	39.23	38.97	10.26	10.18	60.43	60.41	70.69	70.59
298.15	39.85	39.57	12.71	12.62	61.44	61.41	74.15	74.02
300.00	39.93	39.65	12.88	12.78	61.52	61.49	74.39	74.27
350.00	42.90	42.60	16.94	16.81	63.82	63.77	80.75	80.58
400.00	46.75	46.45	20.42	20.27	66.31	66.25	86.73	86.52
450.00	50.74	50.46	23.57	23.40	68.90	68.82	92.46	92.22
500.00	54.59	54.32	26.48	26.31	71.53	71.43	98.01	97.74
550.00	58.16	57.92	29.20	29.02	74.19	74.07	103.38	103.09
600.00	61.43	61.21	31.75	31.57	76.84	76.70	108.59	108.27
650.00	64.41	64.21	34.15	33.96	79.47	79.33	113.62	113.29
700.00	67.12	66.94	36.41	36.22	82.09	81.93	118.50	118.15
750.00	69.58	69.42	38.54	38.35	84.67	84.50	123.21	122.85
800.00	71.84	71.69	40.55	40.37	87.23	87.04	127.78	127.41
850.00	73.90	73.76	42.45	42.27	89.74	89.54	132.19	131.82
900.00	75.78	75.66	44.25	44.07	92.22	92.01	136.47	136.09
950.00	77.51	77.40	45.96	45.78	94.66	94.44	140.62	140.22
1000.00	79.11	79.00	47.58	47.40	97.06	96.83	144.63	144.24
1050.00	80.57	80.48	49.11	48.95	99.42	99.18	148.53	148.13
1100.00	81.92	81.83	50.57	50.41	101.73	101.49	152.31	151.90

Table I (continued)

Temp. (K)	C_p (cal g^{-1} mole^{-1} K^{-1})		$(H-H_0)/T$ (cal g^{-1} mole^{-1} K^{-1})		$-(F-H_0)/T$ (cal g^{-1} mole^{-1} K^{-1})		S (cal g^{-1} mole^{-1} K^{-1})	
	A	B	A	B	A	B	A	B
1150.00	83.17	83.09	51.96	51.80	104.01	103.76	155.98	155.57
1200.00	84.32	84.25	53.29	53.13	106.25	106.00	159.54	159.13
$P=8.0$ atm								
451.00	53.12	52.84	22.50	22.34	67.93	67.85	90.43	90.19
522.70	57.72	57.47	27.02	26.84	71.59	71.48	98.60	98.32
273.15	49.57	49.31	5.12	5.05	60.74	60.72	65.86	65.76
298.15	47.81	47.53	8.77	8.67	61.35	61.32	70.12	69.99
300.00	47.74	47.46	9.01	8.91	61.41	61.38	70.41	70.29
350.00	47.82	47.52	14.51	14.38	63.23	63.18	77.74	77.57
400.00	50.04	49.75	18.80	18.65	65.46	65.39	84.25	84.04
450.00	53.06	52.78	22.43	22.27	67.88	67.80	90.32	90.07
500.00	56.27	56.01	25.66	25.48	70.42	70.32	96.07	95.80
550.00	59.42	59.18	28.58	28.40	73.00	72.88	101.58	101.29
600.00	62.40	62.18	31.28	31.09	75.61	75.47	106.88	106.57
650.00	65.17	64.97	33.78	33.59	78.21	78.06	111.99	111.66
700.00	67.73	67.55	36.12	35.93	80.80	80.64	116.91	116.57
750.00	70.08	69.92	38.30	38.12	83.37	83.19	121.67	121.31
800.00	72.25	72.10	40.36	40.17	85.90	85.72	126.26	125.89
850.00	74.24	74.10	42.29	42.11	88.41	88.21	130.70	130.32
900.00	76.07	75.95	44.12	43.94	90.88	90.67	135.00	134.61
950.00	77.76	77.65	45.85	45.67	93.31	93.09	139.16	138.77
1000.00	79.32	79.21	47.48	47.31	95.70	95.48	143.19	142.79
1050.00	80.75	80.66	49.03	48.86	98.06	97.82	147.09	146.69
1100.00	82.08	81.99	50.50	50.34	100.37	100.13	150.88	150.47
1150.00	83.31	83.23	51.90	51.74	102.65	102.40	154.55	154.14
1200.00	84.44	84.37	53.24	53.08	104.89	104.63	158.12	157.71

DISCUSSION

For real fluids, the non-vanishing molecular size, intermolecular potential fields and molecular motions (chiefly vibrational and rotational modes of motion) contribute greatly to deviations from the ideal gas law

$$PV=RT \tag{2}$$

for one mole of gas.

Assuming that these interactions can be principally described by the molecular

TABLE 2

Calculated constants a, b, c, d and e in eqn. (1)
All values of constants are in cal g^{-1} mole^{-1} K^{-1}.

Assignment	Pressure (atm)	C_p				
		a	b	$c\times10^{-3}$	$d\times10^{7}$	$e\times10^{-11}$
Set A	0.25	−14.97974	0.2006360	−0.1547066	0.5242960	−0.4501119
	0.50	−11.92462	0.1857035	−0.1273145	0.3045134	0.1970830
	1.00	−5.815175	0.1558437	−0.07254165	−0.1349469	1.4911270
	2.00	6.403311	0.09612715	0.03699692	−1.0137970	4.078984
	4.00	30.841830	−0.02331655	0.25609810	−2.771730	9.255484
	8.00	79.721150	−0.2622194	0.6943361	−6.287913	19.609430
Set B	0.25	−14.729970	0.19691410	−0.14616630	0.4497674	−0.2221812
	0.50	−11.675070	0.18198300	−0.11877680	0.2300056	0.4249556
	1.00	−5.565381	0.15212150	−0.06400028	−0.2094898	1.7191180
	2.00	6.653843	0.09240013	0.04554910	−1.0884390	4.307295
	4.00	31.09288	−0.02704761	0.2646602	−2.8464780	9.4841680
	8.00	79.97066	−0.2659401	0.7028752	−6.362445	19.837420

Assignment	Pressure (atm)	S				
		a	$b\times10^{-1}$	$c\times10^{-4}$	$d\times10^{-7}$	$e\times10^{-10}$
Set A	0.25	50.45290	0.9783405	0.4572379	−0.6444731	0.2063844
	0.50	48.05731	1.0281010	0.3659652	−0.57124890	0.1848234
	1.00	44.64330	1.127640	0.1833760	−0.42475070	0.1416852
	2.00	39.19286	1.3267080	−0.1817768	−0.13177750	0.05541585
	4.00	29.66933	1.7248530	−0.9121193	0.4542084	−0.1171374
	8.00	11.99864	2.5212090	−2.372949	1.6263140	−0.4622862
Set B	0.25	50.790530	0.9562260	0.4838240	−0.6596480	0.2097426
	0.50	48.394870	1.0059920	0.3925367	−0.5864056	0.1881752
	1.00	44.980820	1.1055350	0.2099399	−0.4399030	0.1450357
	2.00	39.530170	1.3046160	−0.15524750	−0.14689450	0.05875387
	4.00	30.006590	1.7027610	−0.88558370	0.4390797	−0.1137939
	8.00	12.337110	2.4990310	−2.3462000	1.6109640	−0.4588646

Assignment	Pressure (atm)	$(H-H_0)/T$				
		a	$b\times10^{-1}$	$c\times10^{-4}$	$d\times10^{-7}$	$e\times10^{-10}$
Set A	0.25	0.5663702	0.4748877	0.3209464	−0.491347	0.1664226
	0.50	−0.9552970	0.5493517	0.1842984	−0.3816885	0.1341284
	1.00	−3.998314	0.6982607	−0.08896103	−0.1624001	0.06954856
	2.00	−10.08485	0.9961098	−0.6355447	0.2762322	−0.05962781
	4.00	−22.25726	1.591768	−1.728614	1.153403	−0.3179502
	8.00	−46.60365	2.783183	−3.914977	2.907959	−0.8346622
Set B	0.25	0.8507134	0.4543352	0.3534948	−0.5136305	0.1721531
	0.50	−0.6709471	0.5287986	0.2168478	−0.4039717	0.1398590
	1.00	−3.713973	0.6777072	−0.05641142	−0.1846838	0.07527934
	2.00	−9.800449	0.9755546	−0.6029927	0.2539482	−0.05389756
	4.00	−21.97311	1.571229	−1.696100	1.131155	−0.3122318
	8.00	−46.31966	2.7626656	−3.882502	2.885747	−0.8289551

Assignment	Pressure (atm)	$-(F-H_0)/T$				
		a	$b\times10^{-1}$	$c\times10^{-4}$	$d\times10^{-7}$	$e\times10^{-11}$
Set A	0.25	49.88649	0.5034572	0.1362871	−0.1531245	0.3996118
	0.50	49.01247	0.4787596	0.1816494	−0.1895456	0.5069059
	1.00	48.64143	0.4293932	0.2723093	−0.2623251	0.7212820
	2.00	49.27739	0.3306209	0.4537147	−0.4079622	1.150290
	4.00	51.92645	0.1330955	0.8164768	−0.6991831	2.2008105
	8.00	58.60223	−0.2619737	1.542050	−1.281682	3.723950
Set B	0.25	49.93956	0.5019067	0.1303032	−0.1459997	0.3758441
	0.50	49.06570	0.4771998	0.1756844	−0.1824362	0.4831831
	1.00	48.69473	0.4278309	0.2663491	−0.2552197	0.6975704
	2.00	49.33052	0.3290663	0.4477386	−0.4008435	1.126539
	4.00	51.97978	0.1315296	0.8105258	−0.6920885	1.984439
	8.00	58.65546	−0.2635317	1.536079	−1.274566	3.700200

van der Waals forces. then for low pressures and sufficiently high temperatures it is possible to approximate this fluid behavior by the second term virial expression of eqn. (2) as

$$PV = RT + BT \tag{3}$$

where $B = B(T)$ and is the second virial coefficient. While on one hand the second virial coefficient temperature dependency could be obtained through the choice of a reasonable intermolecular potential function (for instance. Lennard-Jones), it is felt to be more advantageous to express this temperature dependency in terms of corresponding states. Noting the successful application of the Berthelot state equation to fluorobenzene thermodynamic property calculation [3], this simple, two constant equation of state was used also for this work. Indeed, the second virial coefficient [eqn. (3)] may be expressed through Berthelot's equation of state as

$$B = \frac{9}{128} \frac{RT_c}{P_c} \left[1 - 6 \left(\frac{T_c}{T} \right)^2 \right] \tag{4}$$

where the gas constant $R = 82.06$ cm^3 atm K^{-1} and the other entities are in compatible units. The differences between the ideal gas thermodynamic functions (Table 1) and the Berthelot fluid properties, valid for low to moderate pressures up to 8 atm. can be obtained through the application of the following equation set (5) which connects P–V–T properties of the gas to the desired thermodynamic functions.

$$\left(\frac{\partial H}{\partial P} \right)_T = V - T \left(\frac{\partial V}{\partial T} \right)_P; \ \left(\frac{\partial S}{\partial V} \right)_T = \left(\frac{\partial P}{\partial T} \right)_V \tag{5}$$

$$\left(\frac{\partial S}{\partial P} \right)_T = - \left(\frac{\partial V}{\partial T} \right)_P; \ \left(\frac{\partial C_p}{\partial P} \right)_T = -T \left(\frac{\partial^2 V}{\partial T^2} \right)_P$$

Combining eqns. (3)–(5), we arrive at eqns. (6)–(8), yeilding the Berthelot fluid deviation from the ideal gas state given at 1 atm pressure

$$\frac{(H - H_0^\circ)}{T} = \frac{9}{128} \frac{RT_c}{P_c} \left[1 - 18 \left(\frac{T_c}{T} \right)^2 \right] P \tag{6}$$

$$(C_p - C_p^\circ) = \frac{81}{32} \left(\frac{RT_c^3}{P_c T^3} \right) P \tag{7}$$

$$(S^0 - S)_T = \frac{27}{32} \left(\frac{RT_c^3}{P_c T^3} \right) P + R \ln P \tag{8}$$

where the term $R \ln P$ in eqn. (8) is a correction which must be added to obtain the ideal gas entropy at pressure P provided that this correction has not already been included in the ideal gas S^0 expression. It should be noted that for $P = 1$ atm, $R \ln P = 0$.

The thermodynamic functions presented (Table 1) have been obtained using these different equations [eqns. (6)–(8)].

ACCURACY

Lielmezs et al. [1] have already discussed in detail the accuracy and the range of reliability of the calculated thermodynamic functions for naphthalene. They critically compared the results obtained with available experimental and calculated data. They chiefly considered four types of error: mathematical errors due to the round-off in the computer; errors in bond lengths, bond angles and in geometrical asymmetry of the molecule; errors in frequency assignments such as an improper analysis, liquid state frequency shifts; and errors due to the inapplicability of the basic assumptions, for instance, the anharmonicity. Lielmezs et al. [1] concluded that for naphthalene the calculated ideal gas state thermodynamic function's (both assignment sets A and B) uncertainties should be well within the ±0.5% variation up to temperatures of 1000 K.

The calculation of real gas thermodynamic properties additionally, however, involves [eqns. (4), (6)–(8)] the knowledge of the critical state: the critical pressure P_c, and the critical temperature T_c. For naphthalene, the values of the critical parameters [4] are fairly secure. It is expected that the overall error for the calculated real gas values should be within the ±1.0% range. Indirectly, this estimate is supported by the work of Butler and Lielmezs [3] who showed that, for fluorobenzene, the calculated Berthelot gas heat capacities did fit the experimental data of Scott et al. [5] over a pressure range 0.25–10 atm.

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NOMENCLATURE

B = second virial coefficient, cm^3 mole^{-1}
C_p = heat capacity, cal g^{-1} K^{-1}
e.u. = entropy unit, cal g^{-1} mole^{-1} K^{-1}
$-(F-\mathrm{H}_0)/T$ = free energy function, cal g^{-1} mole^{-1} K^{-1}
$(H-H_0)/T$ = enthalpy function
P = pressure, atm
R = universal gas constant
S = entropy, e.u.
T = temperature, K
V = volume, cm^3 g^{-1} mole^{-1}

Superscript

$^\circ$ = reference state referring to the hypothetical state of an ideal gas at 1 atm.

Subscript

c = critical state

p = pressure

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