Thermochimica Acta, 24 (1978) 55–68

THERMODYNAMIC FUNCTIONS OF β-HALONAPHTHALENES FROM 0.25 TO 16 ATMOSPHERES

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(Received 22 June 1977)

ABSTRACT

Real gas thermodynamic functions, C_p, S, $(H - H_o)/T$, and $-(F - H_o)/T$, have been calculated for β-halonaphthalenes (β − $C_{10}H_7X$, where X = F, Cl, Br, I) from 0.25 to 16 atm within the temperature range of 273.15 K to 1200 K, correcting the thermodynamic property ideal gas values by means of the Berthelot equation of state.

INTRODUCTION

Previously, McFee and Lielmezs[1, 2] have calculated the ideal gas state thermodynamic functions at 1 atm for naphthalene and 11 halogenated naphthalenes[1], and the real gas state thermodynamic functions from 0.25 to 16 atm for α-halonaphthalenes[2] (α-$C_{10}H_7X$, where X = F, Cl, Br, I); both compound series within 273.15 to 1200 K temperature range. In this work, however, the real gas state thermodynamic functions have been calculated for β-halonaphthalenes (β-$C_{10}H_7X$, X = F, Cl, Br, I), again from 0.25 to 16 atm and within the temperature range of 273.15 to 1200 K. The calculated results have been presented in Table 1. These results have also been fitted to give five constant polynomial of the form:

$$A = a + bT + cT^2 + dT^3 + eT^4 \quad (1)$$

where A is the real gas thermodynamic function at temperature T (K). The constants a, b, c, d and e (eqn (1)) have been obtained using linear least squares curve fitting methods[3], and are found in Table 2. The molecular structural data needed for thermodynamic function calculations, have been presented in Table 3.

DISCUSSION

The real gas state thermodynamic functions of β-halonaphthalenes were

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TABLE I

HEAT CAPACITY, ENTHALPY FUNCTION, FREE ENERGY FUNCTION AND ENTROPY

Temp. (°K)	β-Fluoronaphthalene				β-Chloronaphthalene			
	C_p (cal mol^{-1} K^{-1})	$(H-H_0)/T$ (cal mol^{-1} K^{-1})	$-(F-H_0)/T$ (cal mol^{-1} K^{-1})	S (cal mol^{-1} K^{-1})	C_p (cal mol^{-1} K^{-1})	$(H-H_0)/T$ (cal mol^{-1} K^{-1})	$-(F-H_0)/T$ (cal mol^{-1} K^{-1})	S cal mol^{-1} K^{-1})
P = 0.25 atm								
451.00	52.03	27.47	81.09	108.56	52.53	27.94	82.69	110.63
522.70	57.99	31.26	85.42	116.67	58.41	31.73	87.09	118.81
273.15	33.29	17.32	70.04	87.36	34.17	17.68	71.43	89.10
298.15	36.15	18.78	71.62	90.40	36.94	19.17	73.04	92.21
300.00	36.36	18.89	71.74	90.63	37.15	19.28	73.16	92.44
350.00	41.95	21.79	74.87	96.66	42.62	22.23	76.35	98.58
400.00	47.18	24.64	77.97	102.60	47.75	25.10	79.51	104.61
450.00	51.94	27.41	81.03	108.44	52.44	27.89	82.63	110.51
500.00	56.31	30.08	84.05	114.14	56.65	30.56	85.70	116.26
550.00	60.01	32.63	87.04	119.68	60.41	33.10	88.74	121.84
600.00	63.41	35.06	89.99	125.05	63.76	35.52	91.72	127.24
650.00	66.44	37.36	92.88	130.24	66.75	37.81	94.66	132.47
700.00	69.15	39.53	95.73	135.27	69.44	39.97	97.54	137.51
750.00	71.60	41.59	98.53	140.12	71.86	42.02	100.37	142.39
800.00	73.81	43.54	101.28	144.82	74.04	43.95	103.14	147.10
850.00	75.81	45.38	103.97	149.35	76.03	45.78	105.86	151.65
900.00	77.63	47.12	106.62	153.74	77.83	47.51	108.53	156.04
950.00	79.30	48.77	109.21	157.98	79.48	49.15	111.14	160.30
1000.00	80.82	50.33	111.75	162.09	80.98	50.71	113.70	164.41
1050.00	82.21	51.82	114.24	166.06	82.36	52.18	116.21	168.40
1100.00	83.49	53.23	116.69	169.92	83.63	53.58	118.67	172.26
1150.00	84.67	54.57	119.08	173.66	84.80	54.92	121.08	176.00
1200.00	85.76	55.85	121.43	177.28	85.88	56.18	123.45	179.63
P = 0.50 atm								
451.00	52.18	27.39	79.73	107.13	52.73	27.84	81.34	109.19
522.70	58.08	31.21	84.05	115.26	58.54	31.67	85.73	117.40
273.15	33.96	16.99	68.77	85.76	35.05	17.24	70.19	87.43
298.15	36.67	18.52	70.33	88.85	37.62	18.84	71.77	90.61
300.00	36.87	18.64	70.44	89.08	37.82	18.95	71.89	90.84
350.00	42.27	21.63	73.54	95.17	43.04	22.02	75.04	97.07
400.00	47.39	24.53	76.62	101.16	48.04	24.97	78.18	103.14
450.00	52.09	27.34	79.67	107.01	52.64	27.79	81.28	109.07
500.00	56.32	30.03	82.69	112.72	56.79	30.48	84.35	114.83
550.00	60.10	32.59	85.68	118.17	60.52	33.05	87.38	120.43
600.00	63.47	35.03	88.62	123.65	63.84	35.48	90.36	125.84
650.00	66.49	37.33	91.51	128.85	66.82	37.78	93.29	131.07
700.00	69.19	39.52	94.36	133.88	69.49	39.95	96.17	136.12
750.00	71.63	41.58	97.16	138.74	71.90	42.00	99.00	141.00
800.00	73.83	43.52	99.91	143.43	74.08	43.94	101.77	145.71
850.00	75.83	45.37	102.60	147.97	76.05	45.77	104.49	150.26
900.00	77.65	47.11	105.24	152.35	77.85	47.50	107.15	154.66
950.00	79.31	48.76	107.83	156.60	79.50	49.14	109.77	158.91
1000.00	80.83	50.33	110.38	160.70	81.00	50.70	112.33	163.03
1050.00	82.22	51.81	112.87	164.68	82.38	52.18	114.84	167.01
1100.00	83.50	53.23	115.31	168.54	83.56	53.58	117.30	170.88
1150.00	84.68	54.57	117.71	172.28	84.81	54.91	119.71	174.62
1200.00	85.76	55.85	120.06	175.90	85.89	56.18	122.07	178.25

β-Bromonaphthalene				β-Iodonaphthalene			
C_p (cal mol^{-1} K^{-1})	$(H-H_0)/T$ (cal mol^{-1} K^{-1})	$-(F-H_0)/T$ (cal mol^{-1} K^{-1})	S (cal mol^{-1} K^{-1})	C_p (cal mol^{-1} K^{-1})	$(H-H_0)/T$ (cal mol^{-1} K^{-1})	$-(F-H_0)/T$ (cal mol^{-1} K^{-1})	S (cal mol^{-1} K^{-1})
52.88	28.56	85.30	113.86	53.07	28.95	87.38	116.33
58.68	32.31	98.79	122.09	58.84	32.67	91.92	124.58
34.85	18.38	73.70	92.08	35.35	18.82	75.56	94.38
37.56	19.88	75.37	95.25	37.98	20.32	77.28	97.59
37.76	19.99	75.49	95.48	38.18	20.43	77.40	97.83
43.12	22.91	78.80	101.71	43.43	23.34	80.77	104.11
48.17	25.76	82.04	107.80	48.41	26.17	84.07	110.24
52.79	28.51	85.24	113.74	52.99	28.90	87.31	116.21
56.94	31.15	88.38	119.53	57.11	31.52	90.49	122.01
60.65	33.67	91.46	125.13	60.80	34.01	93.62	127.63
63.96	36.05	94.50	130.55	64.10	36.39	96.68	133.06
66.91	38.32	97.47	135.79	67.05	38.63	99.68	138.31
69.56	40.46	100.39	140.85	69.70	40.76	102.62	143.38
71.95	42.48	103.25	145.73	72.09	42.77	105.50	148.27
74.10	44.39	106.06	150.44	74.25	44.67	108.32	153.00
76.06	46.19	108.80	154.99	76.21	46.47	111.09	157.56
77.84	47.90	111.49	159.39	78.00	48.17	113.79	161.97
79.47	49.52	114.12	163.65	79.63	49.79	116.44	166.23
80.96	51.06	116.70	167.76	81.12	51.32	119.03	170.35
82.32	52.51	119.23	171.74	82.49	52.77	121.57	174.34
83.58	53.90	121.71	175.60	83.75	54.15	124.06	178.21
84.74	55.21	124.13	179.35	84.91	55.46	126.50	181.96
85.81	56.47	126.51	182.97	85.98	56.71	128.88	185.59
53.08	28.46	83.95	112.42	53.31	28.84	86.04	114.87
58.81	32.24	88.43	120.67	58.99	32.59	96.56	123.16
35.75	17.94	72.47	90.40	36.40	18.30	73.46	92.66
38.25	19.54	74.11	93.64	38.79	19.92	76.03	95.95
38.44	19.65	74.23	93.88	38.97	20.03	76.15	96.19
43.55	22.70	77.49	100.19	43.93	23.09	79.47	102.57
48.46	25.62	80.71	106.33	48.75	26.00	82.75	108.75
52.99	28.41	83.89	112.30	53.22	28.78	85.97	114.75
57.09	31.08	87.02	118.10	57.28	31.43	89.14	120.57
60.76	33.61	90.10	123.72	60.93	33.95	92.26	126.21
64.04	36.01	93.13	129.15	64.20	36.34	95.32	131.65
66.98	38.28	96.11	134.39	67.13	38.60	98.31	136.91
69.62	40.43	99.02	139.45	69.77	40.73	101.25	141.98
71.99	42.46	101.88	144.34	72.14	42.75	104.13	146.88
74.14	44.37	104.68	149.05	74.29	44.65	106.95	151.60
76.09	46.18	107.43	153.61	76.25	46.45	109.71	156.17
77.87	47.89	110.12	158.01	78.03	48.16	112.42	160.58
79.49	49.51	112.75	162.26	79.66	49.78	115.07	164.84
80.98	51.05	115.33	166.38	81.15	51.31	117.66	168.97
82.34	52.51	117.86	170.36	82.51	52.76	120.20	172.96
83.60	53.49	120.33	174.22	83.77	54.14	122.68	176.83
84.75	55.21	122.75	177.96	84.92	55.46	125.12	180.58
85.82	56.46	125.13	181.59	85.99	56.71	127.51	184.21

(Continued on p. 58)

TABLE 1 *(continued)*

HEAT CAPACITY, ENTHALPY FUNCTION, FREE ENERGY FUNCTION AND ENTROPY

Temp.	*β-Fluoronaphthalene*				*β-Chloronaphthalene*			
(°K)	C_p (cal mol^{-1} K^{-1})	$(H-H_0)/T$ (cal mol^{-1} K^{-1})	$-(F-H_0)/T$ (cal mol^{-1} K^{-1})	S (cal mol^{-1} K^{-1})	C_p (cal mol^{-1} K^{-1})	$(H-H_0)/T$ (cal mol^{-1} K^{-1})	$-(F-H_0)/T$ (cal mol^{-1} K^{-1})	S cal mol^{-1} K^{-1})
P = 1.00 atm								
451.00	52.47	27.25	78.40	105.65	53.12	27.65	80.03	107.68
522.70	58.28	31.12	82.71	113.82	58.79	31.54	84.39	115.93
273.15	35.30	16.32	67.62	83.94	36.92	16.36	69.11	85.46
298.15	37.69	18.01	69.12	87.13	38.98	18.16	70.62	88.78
300.00	37.88	18.14	69.23	87.37	39.15	18.29	70.73	89.02
350.00	42.91	21.32	72.27	93.58	43.88	21.61	73.80	95.41
400.00	47.82	24.32	75.31	99.64	48.60	24.69	76.89	101.58
450.00	52.39	27.19	78.34	105.54	53.03	27.59	79.97	107.56
500.00	56.53	29.92	81.35	111.27	57.08	30.34	83.03	113.36
550.00	20.26	32.51	84.32	116.84	60.73	32.94	86.03	118.98
600.00	63.60	34.97	87.26	122.23	64.01	35.40	89.01	124.40
650.00	66.59	37.29	90.15	127.44	66.95	37.71	91.93	129.65
700.00	69.27	39.48	93.00	132.47	69.60	39.90	94.81	134.71
750.00	71.69	41.55	95.79	137.34	71.99	41.96	97.63	139.59
800.00	73.89	43.50	98.53	142.03	74.15	43.90	100.40	144.31
850.00	75.88	45.35	101.23	146.57	76.11	45.74	103.12	148.86
900.00	77.69	47.09	103.87	150.96	77.90	47.48	105.78	153.26
950.00	79.34	48.74	106.46	155.21	79.54	49.13	108.39	157.52
1000.00	80.86	50.32	109.00	159.32	81.04	50.68	110.95	161.64
1050.00	82.25	51.80	111.49	163.30	82.41	52.16	113.46	165.63
1100.00	83.52	53.22	113.94	167.15	83.67	53.57	115.92	169.49
1150.00	84.70	54.56	116.33	170.89	84.84	54.90	118.33	173.23
1200.00	85.78	55.84	118.68	174.52	85.91	56.17	120.70	176.87
P = 2.00 atm								
451.00	53.07	26.96	77.12	104.08	53.90	27.26	78.77	106.04
522.70	58.66	30.93	81.39	112.32	59.29	31.30	83.09	114.39
273.15	37.98	15.00	66.67	81.67	40.36	14.60	68.31	82.91
298.15	39.75	16.99	68.07	85.07	41.71	16.81	69.68	86.49
300.00	39.90	17.14	68.18	85.32	41.83	16.97	69.79	86.75
350.00	44.18	20.69	71.09	91.78	45.56	20.77	72.70	93.47
400.00	48.67	23.90	74.07	97.97	49.73	24.13	75.69	99.82
450.00	52.99	26.90	77.06	103.96	53.82	27.21	78.71	105.92
500.00	56.97	29.71	80.04	109.75	57.66	30.06	81.73	111.79
550.00	60.59	32.36	83.00	115.35	61.17	32.73	84.72	117.45
600.00	63.85	34.85	85.92	120.77	64.34	35.24	87.68	122.91
650.00	66.78	37.19	88.80	126.00	67.21	37.59	90.59	128.18
700.00	69.43	39.40	91.64	131.04	69.81	39.80	93.46	133.26
750.00	71.82	41.49	94.43	135.92	72.16	41.88	96.28	138.16
800.00	73.99	43.45	97.17	140.62	74.29	43.84	99.04	142.88
850.00	75.97	45.31	99.86	145.17	76.23	45.69	101.76	147.44
900.00	77.76	47.06	102.50	149.56	78.00	47.43	104.42	151.85
950.00	79.41	48.72	105.09	153.81	79.62	49.09	107.03	156.11
1000.00	80.91	50.29	107.63	157.92	81.11	50.65	109.59	160.24
1050.00	82.29	51.78	110.12	161.90	82.47	52.13	112.09	164.23
1100.00	83.56	53.20	112.56	165.76	83.73	53.54	114.55	168.09
1150.00	84.73	54.55	114.96	169.50	84.88	54.88	116.96	171.84
1200.00	85.81	55.83	117.31	173.13	85.95	56.15	119.32	175.48

β-Bromonaphthalene				β-Iodonaphthalene			
C_p (cal mol^{-1} K^{-1})	$(H-H_0)/T$ (cal mol^{-1} K^{-1})	$-(F-H_0)/T$ (cal mol^{-1} K^{-1})	S (cal mol^{-1} K^{-1})	C_p (cal mol^{-1} K^{-1})	$(H-H_0)/T$ (cal mol^{-1} K^{-1})	$-(F-H_0)/T$ (cal mol^{-1} K^{-1})	S (cal mol^{-1} K^{-1})
53.47	28.27	82.64	110.91	53.78	38.60	84.73	113.34
59.06	32.12	87.09	119.21	59.29	32.44	89.23	121.68
37.54	17.05	71.38	88.43	38.51	17.25	73.33	90.58
39.63	18.85	72.95	91.80	40.41	19.11	74.92	94.03
39.79	18.98	73.07	92.05	40.56	19.24	75.04	94.28
44.40	22.28	76.25	98.53	44.93	22.60	78.26	100.86
49.03	25.33	79.43	104.76	49.42	25.67	81.48	107.15
53.39	28.21	82.58	110.79	53.69	28.55	84.67	113.22
57.38	30.93	85.69	116.62	57.63	31.26	87.82	119.08
60.98	33.50	88.76	122.27	61.19	33.82	90.92	124.75
64.21	35.93	91.78	127.71	64.40	36.24	93.97	130.21
67.11	38.22	94.75	132.97	67.29	38.52	96.96	135.48
69.72	40.33	97.66	138.04	69.89	40.67	99.89	140.56
72.08	42.41	100.52	142.93	72.25	42.70	102.77	145.47
74.21	44.34	103.32	147.65	74.38	44.61	105.59	150.20
76.15	46.15	106.06	152.21	76.32	46.42	108.35	154.77
77.92	47.87	108.75	156.61	78.09	48.13	111.05	159.18
79.53	49.49	111.38	160.87	79.71	49.75	113.70	163.45
81.01	51.03	113.96	164.99	81.19	51.29	116.29	167.57
82.37	52.49	116.48	168.97	82.55	52.74	118.82	171.57
83.62	53.88	118.96	172.84	83.80	54.13	121.31	175.44
84.78	55.20	121.38	176.58	84.95	55.44	123.75	179.19
85.84	56.45	123.76	180.21	86.02	56.70	126.13	182.83
54.27	27.88	81.39	109.26	54.71	28.14	83.50	111.65
59.57	31.87	85.79	117.66	59.89	32.15	87.95	120.10
41.13	15.26	70.59	85.86	42.72	15.16	72.64	87.79
42.39	17.48	72.03	89.51	43.65	17.50	74.07	91.57
42.50	17.63	72.14	89.77	43.74	17.66	74.18	91.84
46.10	21.43	75.15	96.58	46.93	21.60	77.21	98.81
50.17	24.77	78.23	103.00	50.76	25.01	80.32	105.32
54.19	27.82	81.33	109.14	54.64	28.09	83.44	111.53
57.97	30.65	84.41	115.05	58.31	30.93	86.55	117.48
61.42	33.29	87.45	120.74	61.71	33.57	89.62	123.20
64.55	35.77	90.46	126.22	64.80	36.05	92.65	128.70
67.38	38.09	93.41	131.50	67.60	38.37	95.63	134.00
69.94	40.28	96.31	136.59	70.14	40.55	98.55	139.10
72.25	42.33	99.16	141.50	72.45	42.60	101.42	144.02
74.35	44.27	101.96	146.23	74.55	44.53	104.23	148.77
76.27	46.10	104.70	150.79	76.46	46.35	106.99	153.34
78.02	47.82	107.38	155.20	78.21	48.08	109.69	157.76
79.62	49.45	110.01	159.46	79.81	49.71	112.33	162.04
81.09	51.00	112.59	163.59	81.27	51.25	114.92	166.17
82.44	52.46	115.11	167.58	82.62	52.71	117.46	170.17
83.68	53.85	117.58	171.44	83.87	54.10	119.94	174.04
84.82	55.18	120.01	175.18	85.01	55.42	122.37	177.79
85.88	56.43	122.38	178.82	86.07	56.67	124.76	181.43

(Continued on p. 60)

TABLE 1 *(continued)*

HEAT CAPACITY, ENTHALPY FUNCTION, FREE ENERGY FUNCTION AND ENTROPY

Temp.	*β-Fluoronaphthalene*				*β-Chloronaphthalene*			
(°K)	C_p (*cal mol*$^{-1}$ *K*$^{-1}$)	$(H-H_0)/T$ (*cal mol*$^{-1}$ *K*$^{-1}$)	$-(F-H_0)/T$ (*cal mol*$^{-1}$ *K*$^{-1}$)	S (*cal mol*$^{-1}$ *K*$^{-1}$)	C_p (*cal mol*$^{-1}$ *K*$^{-1}$)	$(H-H_0)/T$ (*cal mol*$^{-1}$ *K*$^{-1}$)	$-(F-H_0)/T$ (*cal mol*$^{-1}$ *K*$^{-1}$)	S *cal mol*$^{-1}$ *K*$^{-1}$)
P = 4.00 atm								
451.00	54.26	26.37	75.93	102.30	55.48	26.49	77.65	104.14
522.70	59.42	30.56	80.13	110.68	60.30	30.80	81.87	112.67
273.15	43.33	12.34	66.17	78.51	47.44	11.08	68.09	79.17
298.15	43.87	14.96	67.36	82.32	47.15	14.11	69.19	83.30
300.00	43.94	15.13	67.46	82.59	47.17	14.32	69.28	83.59
350.00	46.73	19.43	70.12	89.55	48.92	19.11	71.86	90.97
400.00	50.38	23.07	72.96	96.03	51.98	24.02	74.68	97.70
450.00	54.18	26.31	75.87	102.18	55.41	26.43	77.59	104.01
500.00	57.84	29.28	78.80	108.08	58.81	29.50	80.53	110.03
550.00	61.24	32.04	81.72	113.76	62.03	32.31	83.48	115.79
600.00	64.35	34.60	84.62	119.22	65.01	34.91	86.40	121.31
650.00	67.18	37.00	87.48	124.49	67.74	37.33	89.29	126.63
700.00	69.75	39.25	90.31	129.56	70.23	39.60	92.14	131.74
750.00	72.08	41.36	93.09	134.45	72.50	41.72	94.95	136.66
800.00	74.21	43.35	95.82	139.17	74.57	43.71	97.71	141.41
850.00	76.14	45.22	98.51	143.73	76.47	45.58	100.41	145.99
900.00	77.91	46.99	101.14	148.13	78.20	47.34	103.07	150.41
950.00	79.53	48.66	103.73	152.39	79.79	49.01	105.67	154.68
1000.00	81.02	50.24	106.27	156.51	81.25	50.58	108.23	158.81
1050.00	82.39	51.74	108.75	160.50	82.60	52.08	110.73	162.81
1100.00	83.65	53.16	111.19	164.36	83.84	53.49	113.19	166.68
1150.00	84.80	54.51	113.59	168.10	84.98	54.84	115.59	170.43
1200.00	85.87	55.80	115.93	171.73	86.03	56.12	117.96	174.07
P = 8.00 atm								
451.00	56.64	25.21	74.92	100.13	58.62	24.95	76.77	101.71
522.70	60.95	29.82	78.98	108.80	62.32	29.82	80.81	110.62
273.15	54.04	7.03	66.53	73.56	61.59	4.05	69.02	73.07
298.15	52.11	10.88	67.32	78.20	58.03	8.71	69.59	78.30
300.00	52.02	11.13	67.39	78.52	57.85	9.02	69.64	78.66
350.00	51.82	16.92	69.56	86.48	55.65	15.78	71.57	87.35
400.00	53.79	21.39	72.12	93.51	56.49	20.80	74.02	94.82
450.00	56.58	25.14	74.87	100.01	58.57	24.87	76.71	101.58
500.00	59.59	28.43	77.69	106.12	61.12	28.37	79.52	107.88
550.00	62.55	31.40	80.54	111.94	63.77	31.47	82.37	113.83
600.00	65.36	34.12	83.39	117.51	66.35	34.27	85.23	119.49
650.00	67.98	36.62	86.22	122.84	68.79	36.83	88.07	124.90
700.00	70.39	38.95	89.02	127.97	71.07	39.19	90.89	130.08
750.00	72.60	41.12	91.78	132.90	73.18	41.39	93.67	135.05
800.00	74.63	43.15	94.50	137.65	75.13	43.44	96.41	139.85
850.00	76.50	45.06	97.18	142.24	76.94	45.36	99.10	144.45
900.00	78.21	46.85	99.80	146.66	78.60	47.16	101.74	148.90
950.00	79.79	48.55	102.38	150.93	80.13	48.85	104.34	153.19
1000.00	81.24	50.15	104.91	155.06	81.54	50.45	106.88	157.34
1050.00	82.58	51.66	107.40	159.06	82.85	51.96	109.38	161.35
1100.00	83.81	53.09	109.83	162.93	84.05	53.40	111.83	165.23
1150.00	84.95	54.45	112.22	166.68	85.17	54.75	114.24	168.99
1200.00	86.00	55.75	114.57	170.31	86.20	56.04	116.60	172.64

β-Bromonaphthalene				β-Iodonaphthalene			
C_p (cal mol^{-1} K^{-1})	$(H-H_0)/T$ (cal mol^{-1} K^{-1})	$-(F-H_0)/T$ (cal mol^{-1} K^{-1})	S (cal mol^{-1} K^{-1})	C_p (cal mol^{-1} K^{-1})	$(H-H_0)/T$ (cal mol^{-1} K^{-1})	$-(F-H_0)/T$ (cal mol^{-1} K^{-1})	S (cal mol^{-1} K^{-1})
55.87	27.09	80.26	107.36	56.58	27.22	82.43	109.65
60.60	31.37	84.57	115.94	61.09	31.56	86.76	118.32
48.31	11.70	70.39	82.09	51.15	10.97	72.64	83.61
47.91	14.74	71.55	86.29	50.13	14.29	73.75	88.04
47.92	14.95	71.64	86.59	50.10	14.51	73.84	88.35
49.52	19.75	74.32	94.07	50.94	19.62	76.48	96.10
52.46	23.64	77.22	100.86	53.44	23.68	79.37	103.05
55.80	27.03	80.20	107.23	56.52	27.16	82.36	109.52
59.14	30.07	83.21	113.28	59.69	30.25	85.39	115.64
62.30	32.86	86.21	119.07	62.74	33.07	88.41	121.47
65.23	35.41	89.18	124.62	65.59	35.66	91.40	127.06
67.91	37.83	92.11	129.95	68.23	38.07	94.35	132.41
70.36	40.07	95.00	135.07	70.64	40.31	97.25	137.56
72.60	42.17	97.84	140.00	72.86	42.41	100.10	142.51
74.64	44.13	100.62	144.75	74.88	44.37	102.90	147.28
76.51	45.98	103.35	149.34	76.74	46.22	105.65	151.87
78.22	47.28	106.03	153.76	78.44	47.97	108.34	156.31
79.79	49.37	108.66	158.03	80.01	49.61	110.98	160.59
81.23	50.98	111.23	162.16	81.45	51.17	113.57	164.73
82.56	52.41	113.75	166.16	82.77	52.64	116.10	168.74
83.79	53.81	116.22	170.03	83.99	54.04	118.58	172.62
84.92	55.13	118.64	173.78	85.12	55.37	121.01	176.38
85.97	56.40	121.02	177.41	86.16	56.63	123.39	180.02
59.05	25.52	79.39	104.92	60.33	25.38	81.64	107.02
62.65	30.37	83.52	113.88	63.50	30.38	85.76	116.14
62.66	4.56	71.36	75.92	67.99	2.59	74.03	76.62
58.95	9.26	71.97	81.23	63.08	7.85	74.49	82.34
58.75	9.57	72.03	81.60	62.82	8.19	74.54	82.73
56.34	16.37	74.05	90.41	58.95	15.65	76.40	92.05
57.03	21.39	76.57	97.96	58.81	21.03	78.86	99.89
59.01	25.45	79.34	104.78	60.29	25.30	81.59	106.89
61.48	28.93	82.20	111.13	62.43	28.90	84.44	113.35
64.06	32.00	85.10	117.11	64.80	32.06	87.35	119.41
66.58	34.78	88.01	122.79	67.18	34.89	90.26	125.15
68.98	37.32	90.90	128.21	69.48	37.46	93.16	130.62
71.21	39.66	93.75	133.41	71.64	39.83	96.02	135.85
73.29	41.84	96.56	138.39	73.67	42.02	98.85	140.85
75.21	43.86	99.32	143.19	75.55	44.05	101.62	145.68
76.98	45.76	102.04	147.80	77.30	45.96	104.35	150.31
78.62	47.54	104.71	152.25	78.91	47.74	107.03	154.77
80.13	49.22	107.32	156.54	80.41	49.42	109.66	159.08
81.52	50.80	109.89	160.69	81.79	51.01	112.23	163.24
81.81	52.29	112.40	164.69	83.07	52.51	114.76	167.26
84.01	53.71	114.87	168.57	84.25	53.92	117.23	171.16
85.11	55.05	117.29	172.33	85.35	55.26	119.66	174.92
86.13	56.32	119.66	175.98	86.36	56.54	122.04	178.58

(Continued on p. 62)

(TABLE 1 *(continued)*

HEAT CAPACITY, ENTHALPY FUNCTION, FREE ENERGY FUNCTION AND ENTROPY

Temp. (°K)	*β-Fluoronaphthalene*				*β-Chloronaphthalene*			
	C_p (cal mol^{-1} K^{-1})	$(H-H_0)/T$ (cal mol^{-1} K^{-1})	$-(F-H_0)/T$ (cal mol^{-1} K^{-1})	S (cal mol^{-1} K^{-1})	C_p (cal mol^{-1} K^{-1})	$(H-H_0)/T$ (cal mol^{-1} K^{-1})	$-(F-H_0)/T$ (cal mol^{-1} K^{-1})	S cal mol^{-1} K^{-1})
P = 16.00 atm								
451.00	61.40	22.88	74.29	97.17	64.91	21.86	76.38	98.24
522.70	64.01	28.33	78.07	106.40	66.36	27.84	80.06	107.90
273.15	75.46	−3.60	68.64	65.04	89.89	−10.01	72.27	62.26
298.15	68.57	2.72	68.61	71.33	79.80	−2.90	71.75	69.67
300.00	68.19	3.12	68.63	71.75	79.21	−1.59	71.74	70.16
350.00	62.00	11.89	69.82	81.71	69.11	9.12	72.36	81.49
400.00	60.61	18.04	71.83	89.86	65.50	16.35	74.08	90.43
450.00	61.37	22.80	74.24	97.03	64.90	21.76	76.33	98.09
500.00	63.08	26.73	76.85	103.58	65.74	26.11	78.86	104.97
550.00	65.18	30.13	79.56	109.69	67.23	29.78	81.52	111.30
600.00	67.38	33.14	82.31	115.46	69.02	32.97	84.25	117.22
650.00	69.57	35.86	85.07	120.94	70.89	35.82	87.01	122.82
700.00	71.66	38.35	87.82	126.17	72.75	38.39	89.76	128.14
750.00	73.63	40.63	90.55	131.18	74.55	40.74	92.49	133.23
800.00	75.49	42.75	93.24	135.99	76.26	42.91	95.19	138.09
850.00	77.21	44.73	95.89	140.62	77.87	44.92	97.85	142.76
900.00	78.81	46.58	98.50	145.08	79.39	46.79	100.47	147.26
950.00	80.30	48.32	101.07	149.38	80.80	48.54	103.05	151.59
1000.00	81.68	49.95	103.59	153.54	82.12	50.19	105.58	155.77
1050.00	82.95	51.49	106.06	157.55	83.35	51.74	108.07	159.80
1100.00	84.14	52.95	108.49	161.44	84.49	53.20	110.51	163.71
1150.00	85.23	54.33	110.87	165.20	85.55	54.59	112.90	167.49
1200.00	86.25	55.64	113.21	168.85	86.53	55.90	115.25	171.15

calculated in the same manner as those for α-halonaphthalenes[2]; that is, the already calculated[1] ideal gas state thermodynamic property values of β-halonaphthalenes were corrected by means of the second virial coefficient expansion of the Berthelot equation of state. The resulting difference equations given as the real gas deviation from the ideal gas state at one atmosphere pressure, are[2, 4]:

$$(H - H^0)/T = \frac{9}{128}\frac{RT_c}{P_c}\left[1 - 18\left(\frac{T_c}{T}\right)^2\right]P \tag{2}$$

$$(C_p - C_p^0) = \frac{81}{32}\left(\frac{RT_c^3}{P_cT^3}\right)P \tag{3}$$

$$(S^0 - S) = \frac{27}{32}\left(\frac{RT_c^3}{P_cT^3}\right)P + R\ln P \tag{4}$$

The free energy function (Table 1) is found by subtracting eqn (4) and (2). The term $R \ln P$ (eqn (4)) however is a correction which must be included to obtain the ideal

β-Bromonaphthalene				β-Iodonaphthalene			
C_p (cal mol^{-1} K^{-1})	$(H-H_0)/T$ (cal mol^{-1} K^{-1})	$-(F-H_0)/T$ (cal mol^{-1} K^{-1})	S (cal mol^{-1} K^{-1})	C_p (cal mol^{-1} K^{-1})	$(H-H_0)/T$ (cal mol^{-1} K^{-1})	$-(F-H_0)/T$ (cal mol^{-1} K^{-1})	S (cal mol^{-1} K^{-1})
65.43	22.39	79.03	101.41	67.81	21.69	81.46	103.15
66.74	28.36	82.78	111.14	68.31	28.03	85.14	113.16
91.37	−9.71	74.68	64.98	101.69	−14.16	78.17	64.01
81.02	−1.70	74.20	72.50	88.99	−5.02	77.34	72.32
80.42	−1.19	74.19	73.00	88.25	−4.44	77.31	72.87
69.98	9.61	74.88	84.49	74.96	7.72	77.62	85.33
66.17	16.87	76.66	93.54	69.54	15.73	79.20	94.93
65.43	22.29	78.98	101.27	67.82	21.59	81.41	103.00
66.16	26.63	81.56	108.19	67.93	26.21	83.93	110.14
67.57	30.29	84.27	114.56	68.93	30.04	86.61	116.66
69.29	33.46	87.04	120.51	70.36	33.34	89.37	122.71
71.11	36.29	89.84	126.13	71.98	36.25	92.16	128.41
72.92	38.84	92.62	131.46	73.65	38.86	94.94	133.80
74.68	41.17	95 38	136.55	75.30	41.24	97.71	138.94
76.35	43.32	98.11	141.43	76.89	43.41	100.44	143.85
77.94	45.31	100.80	146.11	78.42	45.43	103.13	148.56
79.42	47.16	103.44	150.60	79.86	47.30	105.78	153.08
80.81	48.90	106.04	154.93	81.21	49.05	108.39	157.44
82.11	50.53	108.59	159.11	82.48	50.69	110.94	161.63
83.32	52.06	111.09	163.15	83.66	52.23	113.45	165.69
84.45	53.51	113.54	167.05	84.77	53.69	115.92	169.61
85.50	54.88	115.95	170.83	85.80	55.06	118.34	173.40
86.47	56.17	118.32	174.49	86.76	56.36	120.71	177.07

gas entropy at pressure P, provided that this correction term has not already been included in the ideal gas $S°$-expression.

The applicability of the Berthelot state equation expressed through the second virial coefficient (eqns (2)–(4)) has been in detail discussed by Butler and Lielmezs[4] for fluorobenzene; and by McFee and Lielmezs[2] for α-halonaphthalenes. Indeed, similarly to α-halonaphthalenes[2]; there are no available experimental data for β-halonaphthalenes; and so the accuracy of the presented results (Tables 1 and 2) and the range of applicability of eqns (2)–(4) must be mostly inferred from the general considerations. Using the previously discussed error estimation methods[1, 2, 4], it is found that for β-halonaphthalenes the calculated ideal gas state thermodynamic functions should be reliable from about 400 to 1000 K; the expected error being well within ± 0.5 to ± 2% error range.

The β-halonaphthalene critical point parameters (critical temperature T_c and critical pressure P_c), needed to calculate the real gas thermodynamic properties (eqns (2)–(4)), were approximated to be the same as those of the corresponding α-halonaphthalene parameters. This assumption should not introduce too large error

TABLE 2

CALCULATED CONSTANTS a, b, c, d AND e IN EQN (1)[a]

Pressure (atm)	*β-Fluoronaphthalene*									
	C_p					$(H - H_0)/T$				
	a	b	$c \times 10^3$	$d \times 10^7$	$e \times 10^{11}$	a	$b \times 10$	$c \times 10^5$	$d \times 10^7$	$e \times 10^{10}$
0.25	−11.34019	0.20436	−0.16969	0.66214	−0.87514	0.27074	0.62601	0.62712	−0.30288	0.11474
0.50	−8.17814	0.18890	−0.14134	0.43467	−0.20532	−1.30405	0.70308	−0.78714	−0.18939	0.08132
1.00	−1.85343	0.15800	−0.08465	−0.02021	1.13413	−4.45344	0.85721	−3.61559	0.03759	0.01447
2.00	10.79342	0.09618	0.02875	−0.92999	3.81310	−10.75212	1.16545	−9.27220	0.49154	−0.11922
4.00	36.08907	−0.02745	0.25553	−2.74957	9.17110	−23.34993	1.78197	−20.58628	1.39950	−0.38662
8.00	86.68158	−0.27472	0.70912	−6.38888	19.88756	−48.54483	3.01496	−43.21297	3.21529	−0.92136
16.00	187.8681	−0.76928	1.61632	−13.66781	41.32177	−98.93634	5.48107	−88.46940	6.84717	−1.99095
	$-(F - H_0)/T$					S				
	a	$b \times 10$	$c \times 10^5$	$d \times 10^7$	$e \times 10^{11}$	a	b	$c \times 10^5$	$d \times 10^7$	$e \times 10^{10}$
0.25	52.64552	0.63708	0.25327	−0.10082	0.29483	52.91606	0.12631	0.88016	−0.40368	0.14422
0.50	51.78877	0.61154	0.72238	−0.13848	0.40575	50.48494	0.13146	−0.06439	−0.32790	0.12190
1.00	51.45309	0.56042	1.66146	−0.21388	0.62790	46.99966	0.14176	1.95409	−0.17629	0.07726
2.00	52.15817	0.45824	3.53798	−0.36453	1.07163	41.40601	0.16237	−5.73436	0.12703	−0.01206
4.00	54.94627	0.25386	7.29178	−0.66589	1.95936	31.59666	0.20358	−13.29387	0.73355	−0.19066
8.00	61.90062	−0.15496	14.80074	−1.26876	3.73532	13.35498	0.28601	−28.41395	1.94672	−0.54790
16.00	77.18449	−0.97243	29.81436	−2.47405	7.28558	−21.75029	0.45085	−58.65230	4.37285	−1.26231
	β-Chloronaphthalene									
	C_p					$(H - H_0)/T$				
	a	b	$c \times 10^3$	$d \times 10^7$	$e \times 10^{11}$	a	$b \times 10$	$c \times 10^5$	$d \times 10^7$	$e \times 10^{11}$
0.25	−9.14167	0.19693	−0.15827	0.57834	−0.64031	−0.11621	0.67376	−0.29837	−0.22895	0.93228
0.50	−4.96308	0.17651	−0.12080	0.27778	0.24473	−2.19889	0.77566	−2.16829	−0.07889	0.49037
1.00	3.39463	0.13566	−0.04587	−0.32344	2.01513	−6.36402	0.97945	−5.90780	0.22120	−0.39338
2.00	20.10956	0.05397	0.10398	−1.52576	5.55549	−14.69432	1.38703	−13.38677	0.82136	−2.16085
4.00	53.54086	−0.10943	0.40371	−3.93065	12.63707	−31.35384	2.20210	−28.34252	2.02147	−5.69490
8.00	120.4023	−0.43622	1.00317	−8.74035	26.80001	−64.67592	3.83247	−58.26016	4.42232	−12.76539
16.00	254.1195	−1.08976	2.20196	−18.35853	55.12186	−131.3186	7.09311	−118.0924	9.22372	−26.90528

TABLE 2 *(continued)*

Pressure	$-(F - H_0)/T$					S				
(atm)	*a*	$b \times 10$	$c \times 10^6$	$d \times 10^8$	$e \times 10^{11}$	*a*	*b*	$c \times 10^5$	$d \times 10^7$	$e \times 10^{10}$
0.25	53.51659	0.660428	0.61936	−0.93131	0.29370	53.40013	0.13342	−0.23667	−0.32207	0.12159
0.50	52.82880	0.62662	6.82779	−1.42968	0.43049	50.63011	0.14023	−1.48506	−0.22191	0.09210
1.00	52.83073	0.55898	19.24811	−2.42677	0.72420	46.46664	0.15384	−3.98302	−0.02148	0.03308
2.00	54.21173	0.42374	44.08280	−4.42035	1.31141	39.51802	0.18107	−8.97742	0.37922	−0.08490
4.00	58.35132	0.15323	93.75327	−8.40755	2.48583	26.99590	0.23554	−18.97018	1.18102	−0.32102
8.00	68.00778	−0.38777	193.0933	−16.38190	4.83467	3.33317	0.34446	−38.94872	2.78394	−0.79301
16.00	88.69946	−0.14699	331.7944	−32.33267	9.53302	−42.61882	0.56232	−78.91194	5.99033	−1.73718
	β-Bromonaphthalene									
	C_p					$(H - H_0)/T$				
	a	*b*	$c \times 10^3$	$d \times 10^7$	$e \times 10^{11}$	*a*	$b \times 10$	$c \times 10^5$	$d \times 10^7$	$e \times 10^{11}$
0.25	−7.35821	0.19089	−0.14934	0.51229	−0.44940	0.61680	0.67768	−0.52081	−0.20802	0.86782
0.50	−3.11993	0.17018	−0.11134	0.20741	0.44836	−1.49570	0.78104	−2.41731	−0.05584	0.41965
1.00	5.35655	0.12875	−0.03535	−0.40234	2.24387	−5.72105	0.98776	−6.21056	0.24856	−0.47678
2.00	22.30858	0.04590	0.11663	−1.62162	5.83408	−14.17155	1.40118	−13.79662	0.85731	−2.26949
4.00	56.21712	−0.11984	0.42065	−4.06103	13.01758	−31.07224	2.22801	−28.96788	2.07471	−5.85450
8.00	124.0291	−0.45127	1.02862	−8.93895	27.38128	−64.87762	3.88197	−59.31878	4.51039	−13.02774
16.00	259.6555	−1.11415	2.24458	−18.69509	56.10972	−132.4796	7.18923	120.0035	9.38000	−27.36797
	$-(F - H_0)/T$					S				
	a	$b \times 10$	$c \times 10^5$	$d \times 10^8$	$e \times 10^{11}$	*a*	*b*	$c \times 10^4$	$d \times 10^7$	$e \times 10^{10}$
0.25	54.76344	0.71385	−0.63413	−0.47631	0.16610	55.38045	0.13915	−0.11458	−0.25566	0.10339
0.50	54.08626	0.67951	−0.00367	−0.98245	0.31520	52.59042	0.14606	−0.24211	−0.15407	0.07348
1.00	54.10858	0.61090	1.25620	−1.99378	0.61308	48.38738	0.15987	−0.49547	0.04921	0.01362
2.00	55.53040	0.47368	3.77562	−4.01611	1.20874	41.35909	0.18749	−1.00207	0.45567	−0.10607
4.00	59.75227	0.19920	8.81550	−8.06167	2.40033	28.67844	0.24273	−2.01557	1.26890	−0.34555
8.00	69.57277	−0.34973	18.894 4	−16.15213	4.78333	4.69820	0.35320	−4.04190	2.89467	−0.82428
16.00	90.59235	−1.44767	39.05392	−32.33439	9.54967	−41.88841	0.57416	−8.09508	6.14667	−1.78186

(TABLE 2 *(continued)*

Pressure	*β-Iodonaphthalene*									
(atm)	C_p					$(H - H_0)/T$				
	a	*b*	$c \times 10^3$	$d \times 10^7$	$e \times 10^{11}$	*a*	$b \times 10$	$c \times 10^5$	$d \times 10^7$	$e \times 10^{11}$
0.25	−5.41882	0.18220	−0.13406	0.39642	−0.12681	1.02564	0.68145	−0.77513	−0.18182	0.78064
0.50	−0.44431	0.15789	−0.08947	0.03861	0.92682	−1.45446	0.80547	−3.00121	−0.00320	0.25462
1.00	9.50508	0.10926	−0.00027	−0.67709	3.03430	−6.41505	1.04815	−7.45424	0.35415	−0.79775
2.00	29.40288	0.01201	0.17812	−2.10830	7.24862	−16.33578	1.53347	−16.35922	1.06872	−2.90206
4.00	69.20186	−0.18251	0.53494	−4.97129	15.67921	−36.17726	2.50411	−34.1689	2.49783	−7.11047
8.00	148.796	−0.57152	1.24853	−10.69666	32.53835	−75.86244	4.44557	−69.79401	5.35670	−15.52996
16.00	307.9871	−1.34958	2.67577	−22.14791	66.25831	−155.2308	8.32829	−141.0376	11.07361	−32.36540
	$-(F - H_0)/T$					S				
	a	$b \times 10$	$c \times 10^4$	$d \times 10^9$	$e \times 10^{13}$	*a*	*b*	$c \times 10^1$	$d \times 10^7$	$e \times 10^{11}$
0.25	55.97325	0.74841	−0.10982	−0.16442	0.84592	56.99904	0.14326	−0.18730	−0.19830	0.86534
0.50	55.41751	0.70815	−0.03591	−0.75768	2.59313	53.96327	0.15136	−0.33599	−0.07900	0.51404
1.00	55.68423	0.62756	0.11205	−0.94537	6.09152	49.26950	0.16757	−0.63332	0.15956	−0.18842
2.00	57.59485	0.46642	0.40792	−4.32022	13.08626	41.25929	0.19999	−1.22796	0.63665	−1.59327
4.00	62.79353	0.14411	0.99967	−9.07013	27.07658	26.61490	0.26483	−2.41751	1.59112	−4.40397
8.00	74.56863	−0.50052	2.18324	−18.57067	55.06007	−1.29440	0.39451	−4.79620	3.49963	−10.02382
16.00	99.49596	−1.78975	4.55025	−37.57020	111.0201	−55.73459	0.65385	−9.55341	7.31647	−21.26297

[a] To avoid large errors in applying eqn. (1); all five constants, *a*, *b*, *c*, *d* and *e*, should be used.

TABLE 3

MOLECULAR PARAMETERS

β-fluoronaphthalene					*β-chloronaphthalene*					*β-bromonaphthalene*					*β-Iodonaphthalene*				
191	147	310	355	422	191	138	280	352	410	191	135	274	355	395	191	122	253	355	386
480	519	522	620	708	478	510	517	605	644	478	502	514	580	630	477	498	515	568	627
747	750	768	795	817	749	746	768	795	817	749	745	765	795	815	737	745	765	794	817
852	862	862	955	218	852	862	862	955	218	849	861	861	954	175	860	860	868	951	154
943	967	955	1025	357	943	967	955	1025	357	937	964	954	1020	274	937	965	951	1022	230
1134	1149	1160	1215	1249	1134	1144	1155	1195	1239	1132	1149	1156	1196	1240	1132	1147	1159	1196	1239
1267	1355	1383	1390	1443	1267	1346	1382	1370	1437	1273	1347	1377	1366	1433	1272	1343	1377	1343	1447
1469	1517	1580	1607	1624	1453	1504	1575	1604	1624	1450	1503	1571	1589	1624	1457	1500	1576	1582	1624
3076	528	2987	3027	3031	3076	399	2987	3027	3031	3076	300	2987	3030	3031	3076	250	2987	3027	3031
3060	3060	3076			3060	3060	3076			3060	3090	3390			3060	3060	3076		
Fundamental frequencies[a], *ν (cm⁻¹)*																			
(1)					(2)					(3)					(4)				
Product of the principal moment of inertia[b] *(g³ cm⁶)*																			
394,367 × 10⁻¹¹⁷					772,005 × 10⁻¹¹⁷					1,726,077 × 10⁻¹¹⁷					2,860,927 × 10⁻¹¹⁷				
Normal boiling point (K)																			
490.15[c]					529.15					554.15					581.15				
Critical temperature[d] *(K)*																			
731.60					807.50					834.50					864.20				
Critical pressure[d] *(atm)*																			
36.10					36.73					39.97					37.82				
Symmetry number, σ																			
1					1					1					1				
Molecular weight																			
146.17					162.62					207.08					254.07				

[a] For frequency selection, see discussion by McFee and Lielmezs[1].

[b] For assumptions involving principal moment of inertia calculations, see McFee and Lielmezs[1].

[c] Estimated, this work, from an experimental value at a lower temperature.

[d] Estimated, this work. Note that any α-halonaphthalene gas is determined from its boiling point. Hence calculated thermodynamic property values (Tables 1 and 2) should be used with reference to the particular boiling point value. Any thermodynamic property value *below* the boiling point would refer to the α-halonaphthalene fictious vapor. This effect is especially noted at higher than 8 atm (Table 1).

in the values of β-halonaphthalene critical point parameters since the molecular weights for α- and β-halonaphthalenes are the same, and the respective measured boiling point values[1, 2] differ less than ± 1%. Following the error analysis of McFee and Lielmezs[2] for real gas thermodynamic function values of α-halonaphthalenes; it is suggested that the calculated real gas thermodynamic function values for β-halonaphthalenes (Tables 1 and 2) should be within an overall error range of ±1–±2%. This error is expected to hold for all pressures between temperatures from 400 to 1000 K.

NOMENCLATURE

A	=	angstrom unit
C_p^o	=	heat capacity, cal mol^{-1} K^{-1}
e.u.	=	entropy unit, cal mol^{-1} K^{-1}
$-(F^o - H_0^o)/T$	=	free energy function, cal mol^{-1} K^{-1}
$(H^o - H_0^o)/T$	=	enthalpy function, where $H_0^o = H^o$ at 0 K, cal mol^{-1} K^{-1}
P	=	pressure, atm
R	=	universal gas constant
S^o	=	entropy, e.u.
T	=	temperature, K
T	=	molecular symmetry number
ν	=	wave number, cm^{-1}

Superscript:

o	=	reference state, referring to the hypothetical state of an ideal gas at 1 atm.

Subscript:

c	=	critical state
p	=	pressure

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