

# Vapor Pressure of Coal Chemicals

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The vapor pressure data on 324 coal compounds are collected and analyzed. The adopted data sets for each substance are weighted and combined to fit into a Cox vapor pressure equation,  $\log_{10}P = (1 - D/T) \times 10^{(A + BT + CT^2)}$  by the least-squares method. The results of the literature review and the evaluated values of coefficients for the vapor pressure equations are presented in separate tables. For ease of presentation, the coal compounds are divided into seven groups, based upon their molecular structures. They are (1) benzene and its derivatives, (2) naphthalene and its derivatives, (3) saturated ring compounds, (4) unsaturated ring compounds, (5) heterocyclic sulfur compounds, (6) heterocyclic nitrogen compounds, and (7) heterocyclic oxygen compounds.

**Key words:** aromatic hydrocarbons; benzene derivatives; coal chemicals; Cox equation; cycloalkanes; cycloalkenes; heterocyclic nitrogen compounds; heterocyclic oxygen compounds; heterocyclic sulfur compounds; naphthalene derivatives; vapor pressure; vapor pressure equation.

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## 1. Introduction

Coal has been used for production of industrial organic chemicals for many years. Benzene, toluene, naphthas, tar acids, pyridine bases, anthracene, etc., are separated from coal tar for syntheses of dyestuffs, explosives, perfumes, and drugs. Products from coal gasification and liquefaction may be employed as feedstocks for the manufacture of various organic chemicals.

For large scale manufacturing of coal chemicals, it is essential to have the best values of the basic physical properties of the coal conversion products. The aim of this work is to collect the experimental vapor pressure data on pertinent coal compounds reported in the literature and to fit the adopted data into a selected vapor pressure equation in a systematic fashion. From these results the missing vapor pressure data for useful coal compounds may be estimated by extrapolation or correlation.

It is known that an average of 70% to 80% of the total carbon in bituminous coal is in the aromatic structure, about 15% to 25% is in hydroaromatic structure, and the remaining is aliphatic carbon. The average cluster making up the overall range contains single rings to perhaps six or seven rings.

The heteroatoms like sulfur, oxygen, and nitrogen in coal appear in many types of structures. About 50% of the sulfur is inorganic, principally pyritic. The organic sulfur atoms may exist in structures such as thioether, dialkyl disulfides, thiopenol, aromatic thioether, and cyclic thioethers. The organic oxygen atoms may appear in rings, carbonyls, ethers, and phenolic hydroxyls; and the nitrogen atoms, in pyridine, pyrrole, etc.

For presentation of our evaluated results, the selected coal compounds were separated into the following groups based upon similarity in molecular structure: (1) benzene and its derivatives, (2) naphthalene and its derivatives, (3) saturated ring compounds, (4) unsaturated ring compounds, (5) heterocyclic sulfur compounds, (6) heterocyclic nitrogen compounds, and (7) heterocyclic oxygen compounds.

## 2. Vapor Pressure Equation

Numerous equations have been proposed for representing vapor pressure data on chemical substances. It seems no one equation for fitting the vapor pressure data on all substances with high accuracy has found universal acceptance among investigators.

In the past, mathematically simple vapor pressure equations were preferred. The adjustable parameters were evaluated by simple graphic or numerical methods. However, in recent years, because of the availability of digital electronic computers, mathematically complex vapor pressure equations provide no difficulty for use.

Basically, the selection of a vapor pressure equation depends on the shape of the vapor pressure curves of the given substance. One mathematical equation cannot fit well all the vapor pressure curves for all chemical substances over the entire temperature range from the low temperature triple point up to the critical point.

Often, vapor pressure data are available only over a li-

imited temperature range well below the critical temperature. A simple three-constant or four-constant equation is used to represent them. Obviously, none of these simple equations would be expected to extrapolate reliably to high temperatures up to the critical point, since equations with as many as 11 constants are usually required for the entire liquid range.

The American Petroleum Institute Research Project 44, now renamed the Thermodynamics Research Center (TRC) Hydrocarbon Project,<sup>2</sup> and the TRC Data Project, Texas A&M University, have adopted the Antoine equation for representing the vapor pressure data on many classes of hydrocarbons and related compounds found in petroleum, and on the other classes of both organic and inorganic substances, respectively.

When the pressure and temperature ranges are small, the Antoine equation,  $\log P = A - B/(t + C)$ , where  $A$ ,  $B$ , and  $C$  are adjustable parameters, is capable of representing the results within the experimental error and is adopted generally for correlation purposes. With recent improvement in vapor pressure measurements, the results obtained have greater precision, accuracy, and wider temperature range. Consequently, better vapor pressure equations are needed to represent the experimental measurements. In Engineering Science Data Unit publications,<sup>8</sup> the vapor pressure data on many classes of chemical substances were represented by Chebyshev equations.

Recently, the Wagner equation<sup>76</sup> was used to correlate and extrapolate the experimental vapor pressure data on aliphatic nitrogen compounds in order to incorporate constraints that ensured that the fitted equation exhibited certain established characteristics. This equation may be employed to fit the vapor pressure data for a wide range of compounds with good accuracy. This vapor pressure equation has been used satisfactorily for interpolation of vapor pressure data between 100 to 200 kPa and the critical point. It provides a new procedure for estimation and extrapolation based upon observed values in a limited range.

For higher molecular weight compounds that have low vapor pressures at room temperature, the vapor pressures often are determined at higher temperatures. The selected vapor pressure equations are used for calculating the enthalpies and entropies of vaporization at 298.15 K. The accuracy of the results obtained depends upon how well the vapor pressure equations extrapolate to lower temperatures.

Osborn and Douslin have employed both the Antoine and Cox vapor pressure equations<sup>19</sup> for presenting the vapor pressure data on hydrocarbons,<sup>34</sup> nitrogen compounds,<sup>35</sup> and sulfur compounds<sup>36</sup> found in petroleum. Cox's equation was selected by researchers in the Bartlesville Energy Technology Center for representing the experimental vapor pressure measurements for numerous petroleum compounds for many years.

Scott and Osborn<sup>20</sup> chose five simple vapor pressure equations for fitting the vapor pressures of several typical chemical compounds. From the results obtained, they concluded that the Cox equation yielded by far the best extrapolation both to lower temperatures and to high temperatures from 448 to 530 K. The two three-constant equations, the

Rankine and the Antoine, produced very poor extrapolations. The other two four-constant equations, the Frost-Kalkwarf and the Cragoe, rendered better extrapolations than the three-constant equations, but definitely were inferior to the Cox equation.

New vapor pressure equations have been proposed by Somayajulu<sup>77</sup> and Borrelli *et al.*<sup>78</sup> The merit of these equations is still under investigation.

The above situation indicates the complexity and confusion involved in choosing an appropriate vapor pressure equation for representing the vapor pressure data on chemical compounds.

In selecting a vapor pressure equation in this work, we emphasized the following points as important criteria: (1) the equation should be reliable for extrapolation, (2) the equation should provide no difficulty for generating derivatives, e.g.,  $dP/dT$  or  $d(\ln P)/d(1/T)$ , (3) the equation has been used by reputable researchers and shown its reliability and usefulness, and (4) the equation can be employed for correlation with molecular structure.

After careful scrutinization and evaluation, we decided to use the Cox equation in this work. That this equation may provide reliable extrapolated vapor pressure values without employing the critical constants of the given compounds is particularly valuable, because for many coal compounds these constants are not available.

### 3. Vapor Pressure Data

The vapor pressure data obtained from the literature were converted to SI units, i.e., temperatures in degrees kelvin (K) and pressure in kilopascals (kPa). The adopted data points for each substance were fitted into a Cox equation:  $\log_{10}P = (1 - D/T) \times 10^{(A + BT + CT^2)}$  by the least-squares method, where the constants  $A$ ,  $B$ ,  $C$ , and  $D$  are adjustable parameters. The constants which yielded the smallest deviations were adopted.

In cases where more than one set of vapor pressure data was available for the given compound, a proper weight factor was applied to the data points in each data set before combining them for a least-squares fit into the Cox equation. The value of the weight factor was assigned on the basis of our assessment of the quality of the experimental work reported. A weight factor of 5 to 10 was assigned to the high quality vapor pressure measurements for fitting into the vapor pressure equation.

For some compounds the adopted vapor pressure data points were computed from the vapor pressure equations reported. In many cases, only the smoothed vapor pressures at selected temperatures were available. Many authors did not mention the uncertainties of their experimental mea-

surements, the purities of their sample materials, or the detailed method of measurements. As expected, the quality of the adopted data points was not uniform.

Evaluating and fitting the reported vapor pressure data into an appropriate equation are complicated tasks. The inconsistent data points revealed by the fitting process should be eliminated. Even in the same data set, the uncertainties of the data points in different temperature ranges may be different.

Only a few extensive vapor pressure measurements on aromatic and polynuclear aromatic coal compounds were available in the recent literature. Some pertinent vapor pressure data on coal related substances have been collected and reported.<sup>2,4,6,8,16,35,41,62,65</sup>

We employed the vapor pressure data reevaluated for coal compounds by authoritative and reputable researchers as reliable sources of information in this work. In our opinion, these vapor pressure values, which did not include the inconsistent original data points, are better values for fitting into a vapor pressure equation for extrapolation and estimation of missing data for coal compounds, which is the principal purpose of the present work.

The adopted vapor pressure data sets were divided into several groups, according to the similarity in the molecular structure of the substances included. Within each group of compounds, the arrangement followed an increasing order of the number of carbon atoms in their molecular formulas.

Table 1 contains the vapor pressure data on benzene and its alkyl derivatives. Similar information for naphthalene and its derivatives, unsaturated ring compounds, sulfur, nitrogen, and oxygen compounds are listed in Tables 2–9, respectively.

The contents of each table are compound number, molecular formula, name of compound, vapor pressure range (in kPa), temperature range (K), number of data points, reference number, author's name, year published, data types and method of measurement, and compilations citing the same data. The last item was included to illustrate the presence of cross references on vapor pressure data.

We classified the reported vapor pressure data into four categories A, B, C, and D. The type A data refer to the experimental vapor pressure data measured by the authors of the reference listed. Previously reported experimental data that have been compiled in the indicated reference belong to class B. Class C represents the calculated vapor pressures from a regressed correlation based upon experimental data. Finally, vapor pressure values predicted from theory are denoted as class D.

The results of our comprehensive literature search are summarized in Tables 1–9. The sources of vapor pressure data adopted for fitting into a Cox equation for each individual substance are described in the next section.



TABLE 1. Vapor pressure data on benzene and its derivatives, (continued)

No.	Formula	Name	Vapor Pressure Range, kPa <sup>a</sup>	Temperature Range, K	Number of Data Points	Reference Number	Authors	Year Published	Data Types and Method of Measurement <sup>b</sup>	References Citing the Same Data
28	C <sub>10</sub> H <sub>14</sub>	1-Methyl-4-isopropylbenzene	1.393 - 200.6	330.3 - 480.3	55	2	TCBP	1978	C	15
			12.026 - 104.55	380.19 - 451.57	7	4	Boublik, T. et al.	1973	B	
			0.121 - 2694.2	299. - 650.	73	8	Eng. Sci. Data Unit	1978	C	
29	C <sub>10</sub> H <sub>14</sub>	1,2-Diethylbenzene	1.331 - 198.2	335.9 - 485.9	55	2	TCBP	1978	C	10, 15, 16
			6.425 - 104.02	369.879 - 457.64	20	4	Boublik, T. et al.	1973	B	
			0.112 - 2901.5	295. - 660.	74	8	Eng. Sci. Data Unit	1978	C	
30	C <sub>10</sub> H <sub>14</sub>	1,3-Diethylbenzene	0.133 - 101.33	298.75 - 449.65	10	41	Stull, D.R.	1947	C	10, 15, 16
			1.427 - 197.3	335.9 - 483.1	54	2	TCBP	1978	C	
			6.423 - 104.02	369.242 - 455.31	20	4	Boublik, T. et al.	1973	B	
31	C <sub>10</sub> H <sub>14</sub>	1,4-Diethylbenzene	0.119 - 2716.8	295. - 650.	72	8	Eng. Sci. Data Unit	1978	C	10, 15, 16
			0.133 - 101.33	294.85 - 455.35	10	41	Stull, D.R.	1947	C	
			1.331 - 196.6	335.9 - 485.9	55	2	TCBP	1978	C	
32	C <sub>10</sub> H <sub>14</sub>	1,2-Dimethyl-3-ethylbenzene	6.422 - 104.02	371.967 - 457.97	20	4	Boublik, T. et al.	1973	B	10, 15, 16
			0.107 - 2708.6	295. - 655.	73	8	Eng. Sci. Data Unit	1978	C	
			0.133 - 101.33	292.55 - 455.65	10	41	Stull, D.R.	1947	C	
33	C <sub>10</sub> H <sub>14</sub>	1,2-Dimethyl-4-ethylbenzene	1.331 - 199.98	344.25 - 497.15	27	2	TCBP	1978	C	10
			0.139 - 2956.5	305. - 675.	75	8	Eng. Sci. Data Unit	1978	C	
			1.331 - 199.98	341.05 - 492.85	27	2	TCBP	1978	C	
34	C <sub>10</sub> H <sub>14</sub>	1,3-Dimethyl-2-ethylbenzene	0.114 - 2858.4	300. - 665.	74	8	Eng. Sci. Data Unit	1978	C	10
			1.358 - 204.8	341.4 - 494.2	56	2	TCBP	1978	C	
			0.112 - 2864.6	300. - 670.	75	8	Eng. Sci. Data Unit	1978	C	
35	C <sub>10</sub> H <sub>14</sub>	1,3-Dimethyl-4-ethylbenzene	1.269 - 199.9	388.7 - 491.4	56	2	TCBP	1978	C	10, 15
			0.130 - 2852.5	300. - 665.	74	8	Eng. Sci. Data Unit	1978	C	
			0.133 - 101.33	296.35 - 457.65	10	41	Stull, D.R.	1947	C	
36	C <sub>10</sub> H <sub>14</sub>	1,3-Dimethyl-5-ethylbenzene	1.310 - 197.2	335.9 - 485.9	55	2	TCBP	1978	C	10, 15
			0.107 - 2633.3	295. - 650.	72	8	Eng. Sci. Data Unit	1978	C	
			0.133 - 101.33	296.35 - 458.15	10	41	Stull, D.R.	1947	C	
37	C <sub>10</sub> H <sub>14</sub>	1,4-Dimethyl-2-ethylbenzene	1.372 - 194.4	338.7 - 488.7	55	2	TCBP	1978	C	10, 15
			0.101 - 3381.6	295. - 680.	78	8	Eng. Sci. Data Unit	1978	C	
			0.133 - 101.33	297.25 - 458.15	10	41	Stull, D.R.	1947	C	
38	C <sub>10</sub> H <sub>14</sub>	1,2,3,4-Tetramethylbenzene	1.331 - 196.5	352.6 - 508.1	57	2	TCBP	1978	C	10, 15
			0.111 - 2970.1	310. - 690.	77	8	Eng. Sci. Data Unit	1978	C	
			0.3401 - 107.31	330. - 480.	16	10	Jordan, T.E.	1954	C	
39	C <sub>10</sub> H <sub>14</sub>	1,2,3,5-Tetramethylbenzene	1.289 - 204.8	347.0 - 502.6	57	2	TCBP	1978	C	10, 15
			0.106 - 2850.3	305. - 675.	75	8	Eng. Sci. Data Unit	1978	C	
			0.3988 - 98.765	330. - 470.	15	10	Jordan, T.E.	1954	C	
40	C <sub>10</sub> H <sub>14</sub>	1,2,4,5-Tetramethylbenzene	1.351 - 198.6	347.0 - 499.8	56	2	TCBP	1978	C	10, 15
			1.996 - 2913.0	355. - 675.	75	8	Eng. Sci. Data Unit	1978	C	
			0.3988 - 98.765	330. - 470.	15	10	Jordan, T.E.	1954	C	
41	C <sub>11</sub> H <sub>16</sub>	sec-Amylbenzene	0.133 - 101.33	300.95 - 451.15	10	41	Stull, D.R.	1947	C	10, 15
42	C <sub>11</sub> H <sub>16</sub>	3-Ethyl-1-isopropylbenzene	0.133 - 101.33	301.45 - 466.15	10	41	Stull, D.R.	1947	C	10, 15
43	C <sub>11</sub> H <sub>16</sub>	4-Ethyl-1-isopropylbenzene	0.133 - 101.33	304.65 - 468.95	10	41	Stull, D.R.	1947	C	10, 15
44	C <sub>11</sub> H <sub>16</sub>	3,5-Diethyltoluene	0.133 - 101.33	304.95 - 472.15	10	41	Stull, D.R.	1947	C	15
45	C <sub>11</sub> H <sub>16</sub>	1,2,4-Trimethyl-5-ethylbenzene	1.467 - 9.466	360.45 - 405.5	11	4	Boublik, T. et al.	1973	C	15
46	C <sub>11</sub> H <sub>16</sub>	1,3,5-Trimethyl-2-ethylbenzene	0.133 - 101.33	316.85 - 481.25	10	41	Stull, D.R.	1947	C	
47	C <sub>12</sub> H <sub>18</sub>	1,2-Diisopropylbenzene	1.573 - 101.33	361.65 - 483.35	19	41	Boublik, T. et al.	1973	B	15, 10, 15
			0.133 - 101.33	311.95 - 481.15	10	41	Stull, D.R.	1947	C	
48	C <sub>12</sub> H <sub>18</sub>	1,3-Diisopropylbenzene	0.133 - 101.33	313.15 - 482.15	10	41	Stull, D.R.	1947	C	10, 15
49	C <sub>12</sub> H <sub>18</sub>	1,4-Diisopropylbenzene	0.133 - 101.33	307.85 - 475.15	10	41	Stull, D.R.	1947	C	10, 15
50	C <sub>12</sub> H <sub>18</sub>	1,2,4-Triethylbenzene	6.753 - 104.63	393.41 - 484.73	7	4	Boublik, T. et al.	1973	B	15
51	C <sub>12</sub> H <sub>18</sub>	1,3,4-Triethylbenzene	0.133 - 101.33	319.15 - 491.15	10	41	Stull, D.R.	1947	C	10, 15
52	C <sub>12</sub> H <sub>18</sub>	Hexamethylbenzene	2.80 x 10 <sup>-6</sup> - 0.014	303.10 - 343.02	2	48	Ambrose, D.	1976	A, static	

<sup>a</sup> 1 kPa = 7.50062 torr (mm Hg)

<sup>b</sup>

A = experimental data measured by the author(s) of the reference.  
 B = experimental data collected from literature by the author(s) of the reference.  
 C = calculated values from a regressed correlation based on experimental data.  
 D = predicted values from theory.

TABLE 2. Vapor pressure data on naphthalene and its derivatives

No.	Formula	Name	Vapor Pressure Range, kPa <sup>a</sup>	Temperature Range, K	Number of Data Points	Reference Number	Authors	Year Published	Data Types and Method of Measurement <sup>b</sup>	Reference Citing the Same Data
1	C <sub>10</sub> H <sub>10</sub>	Naphthalene	1.001 - 38.786	353.48 - 452.66	32	4	Boublik, T. et al.	1973	B	15
			0.00080 - 4045.4	273.15 - 751.65	63	6	Coal Tar Res. Ass.	1965	B	16
			0.28.10 - 0.5253	223.151 - 340.15	13	57	Timmermans, J.	1965	B	
			0.00232 - 110.02	283.15 - 494.60	17	16	Vergátlík, N.B.	1975	B	
			0.0004 - 1337.0	273.2 - 643.2	38	17	Yaws, C.	1978	C	
			1.587 - 110.018	360.62 - 494.60	27	18	Bradley, R.S. et al.	1953	A, Gas Effusion	
			28.82 - 3378.42	441.32 - 727.59	15	22	De Kluif, C.G.	1980	D	
			0.000163 - 0.0007119	279.85 - 293.85	11	23	MacKnight, A.B. et al.	1979	A, Gas-Saturation	
			0.000176 - 0.001	257.21 - 257.21	10	45	Ambrose, D. et al.	1975	A, Static	15
			0.00176 - 0.02053	280.3 - 305.0	22	22	TCHP	1978	C	
			23.10 - 0.4886	263.61 - 343.06	60	22	Jordan, T.F.	1954	C	
			1.413 - 209.5	360.9 - 524.8	60	10	Wilson, G.M., et al.	1981	A, Static	
			1.13 - 4023.94	80.3 - 552.6	73	73	TCHP	1978	C	
			5.524 - 102.765	415.29 - 518.48	63	4	Boublik, T. et al.	1973	B	15
			0.00176 - 0.0235	278.85 - 311.75	8	28	MacKnight, A.B. et al.	1979	A, Gas-Saturation	
7.719 - 415.36	424.43 - 593.38	24	53	Wiczorek, S.A. et al.	1980	A, Static				
15.58 - 3026.79	447.04 - 755.37	18	73	Wilson, G.M., et al.	1981	A, Static				
1.310 - 197.9	377.6 - 547.0	62	2	TCHP	1978	C	15			
5.536 - 102.937	412.34 - 514.91	17	53	Boublik, T. et al.	1973	B				
8.627 - 821.27	424.41 - 638.93	29	29	Wiczorek, S.A. et al.	1980	A, Static				
0.133 - 101.33	343.15 - 531.25	63	2	TCHP	1978	C	10, 15			
1.448 - 205.5	394.2 - 566.4	63	2	TCHP	1978	C				
0.00153 - 0.01999	286.2 - 318.25	7	28	MacKnight, A.B. et al.	1979	A, Gas-Saturation				
1.379 - 112.4	402.6 - 544.2	52	2	TCHP	1978	C				
1.655 - 402.6	402.6 - 541.4	15	2	TCHP	1978	C				
1.310 - 103.99	397.0 - 544.15	16	2	TCHP	1978	C				
0.0148 - 1.8032	328.15 - 413.15	20	38	Osborn, A.G. et al.	1975	A, Ebulliometric	15			
0.0140 - 1.8534	33.15 - 408.15	15	38	Osborn, A.G. et al.	1975	A, Ebulliometric	15			
0.05360 - 3.4419	348.15 - 418.15	15	38	Osborn, A.G. et al.	1975	A, Ebulliometric	15			
0.01987 - 1.5037	333.15 - 398.15	15	38	Osborn, A.G. et al.	1975	A, Ebulliometric	15			
1.333 - 101.33	403.15 - 545.95	10	2	TCHP	1978	C				
1.333 - 101.33	404.15 - 546.65	10	2	TCHP	1978	C				
1.344 - 208.2	402.5 - 577.6	64	2	TCHP	1978	C				
1.393 - 202.7	402.6 - 577.6	64	2	TCHP	1978	C				
0.133 - 101.33	349.15 - 539.15	10	41	Stull, D.R.	1947	C				
1.333 - 101.33	415.15 - 557.65	8	2	TCHP	1978	C				
1.333 - 101.33	409.15 - 553.15	7	2	TCHP	1978	C				
1.333 - 101.33	415.15 - 558.15	7	2	TCHP	1978	C				
1.400 - 107.6	413.7 - 566.4	56	2	TCHP	1978	C				
0.0667 - 1.3332	362.15 - 420.65	5	1	API 42	1966	A				
1.379 - 112.4	419.2 - 566.4	54	2	TCHP	1978	C				
0.0667 - 1.3332	353.15 - 410.65	5	1	API 42	1966	A				
1.379 - 133.8	408.1 - 566.4	58	2	TCHP	1978	C				
0.0667 - 1.3332	351.15 - 408.65	5	1	API 42	1966	A				
1.379 - 128.9	408.1 - 566.4	58	2	TCHP	1978	C				

<sup>a</sup> 1 kPa = 7.5002 torr (mm Hg).

<sup>b</sup> A = experimental data measured by the author(s) of the reference.  
 B = experimental data collected from literature by the author(s) of the reference.  
 C = calculated values from a regressed correlation based on experimental data.  
 D = predicted values from theory.

Table 3. Vapor pressure data on saturated ring compounds

No.	Formula	Name	Vapor Pressure Range, kPa <sup>a</sup>	Temperature Range, K	Number of Data Points	Reference Number	Authors	Year Published	Data Types <sup>b</sup> and Method of Measurement	Reference Citing the Same Data
1	C <sub>3</sub> H <sub>6</sub>	Cyclopropane	1.333-199.98	171.85-257.37	27	2	TRCHP	1978	C	16
			3.50-104.74	181.121-241.067	13	4	Boublik, T. et al	1973	B	
			3.68-5582.11	183.15-398.35	10	18	Yaws, C.	1978	C	
			0.133-101.33	156.4-239.7	24	41	Stull, D.R.	1947	C	
2	C <sub>4</sub> H <sub>8</sub>	Cyclobutane	631.56-5579.46	293.15-398.30	24	54	Lin, D.C.K. et al	1970	A	10
			1.333-199.98	204.95-305.66	27	2	TRCHP	1978	C	
			2.50-100.15	213.220-285.345	12	4	Boublik, T. et al	1973	B	
			0.13-4847.34	181.15-463.55	10	18	Yaws, C.	1978	C	
3	C <sub>4</sub> H <sub>8</sub>	Methylcyclopropane	0.133-101.33	181.2-286.1	10	41	Stull, D.R.	1947	C	10
			0.813-103.192	198.75-286.23	13	70	Hessig, G. B.	1941	A	
			0.133-101.33	177.2-277.7	10	41	Stull, D.R.	1947	C	
			1.333-199.98	232.75-344.75	27	2	TRCHP	1978	C	
4	C <sub>5</sub> H <sub>10</sub>	Cyclopentane	0.83-103.92	225.90-323.18	22	4	Boublik, T. et al	1973	B	10,15,16
			0.080-2.360	193.15-240.65	3	7	Doss, M.P.	1943	B	
			0.043-4039.0	193.2-503.2	33	17	Vargaftik, N.B.	1975	B	
			0.29-4530.30	213.15-511.65	8	18	Yaws, C.	1978	C	
			1.57-4023.4	234.085-503.215	8	50	Pasek, G.J. et al	1962	B	
			5.333-199.98	279.84-378.35	24	2	TRCHP	1978	C	
			5.35-103.92	279.47-354.73	22	4	Boublik, T. et al	1973	B	
			6.33-3561.0	283.2-543.2	28	17	Vargaftik, N.B.	1975	B	
			0.72-4107.80	247.75-553.45	15	18	Yaws, C.	1978	C	
			0.133-3039.	227.85-530.65	6	41	Stull, D.R.	1947	C	
5	C <sub>6</sub> H <sub>12</sub>	Cyclohexane	13.04-85.01	298.-348.	6	46	Cruickshank, A. et al	1967	A, Static	6, 10,16
			936.6-4074.8	451.44-553.69	12	47	Hugill, J. A. et al	1978	A	
			10.25-3959.4	293.165-551.225	8	50	Pasek, G. J. et al	1962	B	
			1.333-199.98	249.45-368.85	27	2	TRCHP	1978	C	
			19.92-270.11	339.354-432.172	15	4	Boublik, T. et al	1973	B	
			14.57-70.07	293.05-330.60	3	7	Doss, M.P.	1943	B	
			0.00185-2924.	183.15-513.15	33	17	Vargaftik, N.B.	1975	B	
			6	C <sub>6</sub> H <sub>12</sub>	Methylcyclopentane					

Table 3. Vapor pressure data on saturated ring compounds--Continued

No.	Formula	Name	Vapor Pressure Range, kPa	Temperature Range, K	Number of Data Points	Reference Number	Authors	Year Published	Data Types <sup>b</sup> and Method of Measurement	Reference Citing the Same Data
7	C <sub>7</sub> H <sub>14</sub>	Cycloheptane	1.333-199.98 19.920-270.111	284.35-418.88 341.334-432.172	27 15	2 4	TRCHP Boublik, T. et al	1978 1973	C B	15
8	C <sub>7</sub> H <sub>14</sub>	Ethylcyclopentane	1.333-199.98 6.41-103.99 1.341-314.3 0.133-101.33	273.24-402.45 301.928-377.532 273.2-563.2 240.95-376.55	27 20 30 10	2 4 17 41	TRCHP Boublik, T. et al Vargaftik, N. B. Stull, D. R.	1978 1973 1975 1947	C B B C	10 10,15
9	C <sub>7</sub> H <sub>14</sub>	1,1-Dimethylcyclopentane	1.333-199.98 6.415-103.99 0.02582-561.37	260.84-388.15 288.648-361.886 213.15-433.15	27 19 24	2 4 17	TRCHP Boublik, T. et al Vargaftik, N. B.	1978 1973 1975	C B B	10 3,15
10	C <sub>7</sub> H <sub>14</sub>	1,cis-2-Dimethylcyclopentane	1.333-199.98 6.41-103.99	271.89-398.35 298.497-379.596	27 20	2 4	TRCHP Boublik, T. et al	1978 1973	C B	10 15
11	C <sub>7</sub> H <sub>14</sub>	1,trans-2-Dimethylcyclopentane	1.333-199.98 8.99-103.99	264.15-390.25 299.263-365.919	27 18	2 4	TRCHP Boublik, T. et al	1978 1973	C B	10 15
12	C <sub>7</sub> H <sub>14</sub>	1,cis-3 Dimethylcyclopentane	1.333-199.98 9.013-104.02	263.15-389.15 299.127-365.778	27 18	2 4	TRCHP Boublik, T. et al	1978 1973	C B	10 15
13	C <sub>7</sub> H <sub>14</sub>	1,trans-3-Dimethylcyclopentane	1.333-199.98 6.41-103.99	263.95-390.15 291.155-364.820	27 19	2 4	TRCHP Boublik, T. et al	1978 1973	C B	10 15
14	C <sub>7</sub> H <sub>14</sub>	Methylcyclohexane	1.333-199.98 6.35-103.92 1.333-199.98 0.0036-3116.0	269.95-400.15 298.736-374.982 269.95-400.15 203.2-563.2	27 20 30 38	2 4 6 17	TRCHP Boublik, T. et al Coal Tar Res. Ass. Vargaftik, N. B.	1978 1973 1965 1975	C B B B	10 10
15	C <sub>8</sub> H <sub>16</sub>	Ethylcyclohexane	1.333-199.98 0.033-310.80 0.133-101.33	293.75-432.65 243.2-453.2 258.65-404.95	27 22 10	2 17 41	TRCHP Vargaftik, N. B. Stull, D. R.	1978 1975 1947	C B C	10
16	C <sub>8</sub> H <sub>16</sub>	1,1-Dimethylcyclohexane	1.333-199.98 6.413-104.00 0.133-101.33	283.25-420.25 313.647-393.670 248.75-392.65	27 20 10	2 4 41	TRCHP Boublik, T. et al Stull, D. R.	1978 1973 1947	C B C	10 15



Table 3. Vapor pressure data on saturated ring compounds--Continued

No.	Formula	Name	Vapor Pressure Range, kPa <sup>a</sup>	Temperature Range, K	Number of Data Points	Reference Number	Authors	Year Published	Data Types <sup>b</sup> and Method of Measurement	Reference Citing the Same Data
17	C <sub>8</sub> H <sub>16</sub>	1, cis-2-Di-methylcyclohexane	1.333-199.98 6.353-103.91 0.133-101.33	291.55-430.75 322.335-403.834 257.3-402.9	27 20 10	2 4 41	TRCHP Boublik, T. et al Stull, D. R.	1978 1973 1947	C B C	10 15
18	C <sub>8</sub> H <sub>16</sub>	1, trans-2-Di-methylcyclohexane	1.333-199.98 0.133-101.33	286.2-424.3 252.1-396.6	27 10	2 41	TRCHP Stull, D. R.	1978 1947	C C	10
19	C <sub>8</sub> H <sub>16</sub>	1, cis-3-Di-methylcyclohexane	1.333-199.98 0.133-101.33	284.4-420.6 253.8-397.6	27 10	2 41	TRCHP Stull, D. R.	1978 1947	C C	3,10 3
20	C <sub>8</sub> H <sub>16</sub>	1, trans-3-Di-methylcyclohexane	1.333-199.98 0.133-101.33	288.1-425.1 250.5-393.3	27 10	2 41	TRCHP Stull, D. R.	1978 1947	C C	3 3
21	C <sub>8</sub> H <sub>16</sub>	1, cis-4-Dimethylcyclohexane	333-199.98 0.133-101.33	287.7-425.0 253.2-397.5	27 10	2 41	TRCHP Stull, D. R.	1978 1947	C C	3 3
22	C <sub>8</sub> H <sub>16</sub>	1, trans-4-Di-methylcyclohexane	1.333-199.98 0.133-101.33	283.2-420.0 248.5-392.5	27 10	2 41	TRCHP Stull, D. R.	1978 1947	C C	
23	C <sub>8</sub> H <sub>16</sub>	Isopropylcyclopentane	6.40-104.00 1.333-199.98	320.183-400.544 289.55-426.95	20 27	4 2	Boublik, T. et al TRCHP	1973 1978	B C	15
24	C <sub>8</sub> H <sub>16</sub>	Propylcyclopentane	6.40-104.00 1.333-199.98	325.025-405.067 294.45-431.35	19 27	4 2	Boublik, T. et al TRCHP	1973 1978	B C	15
25	C <sub>8</sub> H <sub>16</sub>	1-Ethyl-1-methylcyclopentane	6.41-104.00 0.042-270.02 1.333-199.98	316.206-395.634 238.150-435.293 285.85-421.85	20 32 27	4 34 2	Boublik, T. et al Osborn, A.G. et al TRCHP	1973 1947 1978	B A, Ebulliometric C	15
26	C <sub>8</sub> H <sub>16</sub>	cis-2-Ethyl-1-methylcyclopentane	6.40-104.00 0.028-1.114 1.333-199.98	321.996-402.171 238.150-288.150 291.34-428.55	20 11 27	4 34 2	Boublik, T. et al Osborn, A.G. et al TRCHP	1973 1974 1978	B A, Ebulliometric C	15
27	C <sub>8</sub> H <sub>16</sub>	1,1,2-Trimethylcyclopentane	6.41-104.00 1.333-199.98	309.357-387.836 279.55-413.75	19 27	4 2	Boublik, T. et al TRCHP	1973 1978	B C	15
28	C <sub>8</sub> H <sub>16</sub>	1,1,3-Trimethylcyclopentane	6.41-104.00 1.333-199.98	302.094-378.980 272.85-404.45	19 27	4 2	Boublik, T. et al TRCHP	1973 1978	B C	15

Table 3. Vapor pressure data on saturated ring compounds--Continued

No.	Formula	Name	Vapor Pressure Range, kPa <sup>a</sup>	Temperature Range, K	Number of Data Points	Reference Number	Authors	Year Published	Data Types <sup>b</sup> and Method of Measurement	Reference Citing the Same Data
29	C <sub>9</sub> H <sub>18</sub>	Propylcyclohexane	6.41-104.00 1.333-199.98	345.841-430.906 313.35-458.95	20 27	4 2	Boublik, T. et al TRCHP	1973 1978	B C	10 3
30	C <sub>9</sub> H <sub>18</sub>	Isopropylcyclohexane	6.411-104.01	343.665-428.752	20	4	Boublik, T. et al	1973	B	
31	C <sub>9</sub> H <sub>18</sub>	cis-3-Ethyl-1-methylcyclohexane	9.588-269.980	348.306-464.422	21	34	Osborn, A.G. et al	1974	A, Ebulliometric	
32	C <sub>9</sub> H <sub>18</sub>	1,1,3 - Trimethylcyclohexane	6.398-104.00	327.819-410.786	20	4	Boublik, T. et al	1973	B	50
33	C <sub>10</sub> H <sub>20</sub>	n-Butylcyclohexane	1.333-199.98	332.65-484.35	27	2	TRCHP		C	
34	C <sub>10</sub> H <sub>20</sub>	Isobutylcyclohexane	6.41-104.01	357.902-445.544	20	4	Boublik, T. et al	1973	B	8
35	C <sub>10</sub> H <sub>20</sub>	sec-Butylcyclohexane	6.41-104.01	367.606-453.571	20	4	Boublik, T. et al	1973	B	
36	C <sub>10</sub> H <sub>20</sub>	tert-Butylcyclohexane	6.40-104.00	357.183-445.820	20	4	Boublik, T. et al	1973	B	

<sup>a</sup> 1 kPa = 7.50062 torr (mmHg)<sup>b</sup> A = Experimental Data Measured by the Author(s) of the Reference.

B = Experimental Data Collected from Literature by the Author(s) of the Reference.

C = Calculated Values from a Regressed Correlation Based on Experimental Data.

Table 4. Vapor pressure data on unsaturated ring compounds

No.	Formula	Name	Vapor Pressure Range, kPa	Temperature Range, K	Number of Data Points	Reference Number	Authors	Year Published	Data Types <sup>b</sup> and Method of Measurement	Reference Citing the Same Data
1	C <sub>4</sub> H <sub>6</sub>	Cyclobutene	1.160-98.939 0.133-101.33	196.050-275.050 174.1-275.6	12 10	70 41	Heisig, G. B. Stull, D. R.	1941 1947	A C	4,10,15
2	C <sub>5</sub> H <sub>6</sub>	1,3-Cyclopentadiene	18.821-96.327	271.25-313.05	6	15	Shuzo, O.	1978	B	
3	C <sub>5</sub> H <sub>8</sub>	Cyclopentene	0.85-743.80 1.447-39.89	223.2-393.2 230.40-292.92	18 4	17 71	Vargaftik, N. B. Lister, M. W.	1975 1941	B A, Static	
4	C <sub>6</sub> H <sub>8</sub>	1,3-Cyclohexadiene	16.8-34.76 307.34-363.31	303.96-322.03 19,444-135.198	7 12	27 41	Letcher, T.M. et al Meyer, E. F. et al	1974 1973	A, Static A, Ebulliometric	15
5	C <sub>6</sub> H <sub>8</sub>	1,4-Cyclohexadiene	11.89-25.25	304.25-322.23	7	27	Letcher, T.M. et al	1974	A, Static	
6	C <sub>6</sub> H <sub>10</sub>	Cyclohexene	0.033-528.70 16.29-32.25 19.885-129.633 0.160-0.752	213.2-423.2 305.37-322.14 310.03-364.53 228.73-248.30	22 7 10 4	17 27 31 71	Vargaftik, N. B. Letcher, T. M. et al Meyer, E. F. et al Lister, M. W.	1975 1974 1973 1941	B A, Static A, Ebulliometric A, Static	15
7	C <sub>9</sub> H <sub>8</sub>	Indene	0.133-104.41 0.133-101.33	289.55-456.97 289.6-454.8	10 10	6 41	Coal Tar Res. Ass. Stull, D. R.	1965 1947	B C	10
8	C <sub>9</sub> H <sub>10</sub>	Indan	6.623-104.44 4.343-206.401 9.59-143.24	364.83-452.24 355.006-482.437 374.274-465.558	7 25 19	6 26 37	Coal Tar Res. Ass. Ambrose, D. et al Osborn, A.G. et al	1965 1976 1978	B A, Ebulliometric A, Ebulliometric	
9	C <sub>10</sub> H <sub>12</sub>	Tetralin	2.67-98.66 1.74-348.03 0.133-101.33 46.47-3364.64	366.950-479.350 355.44-540.35 311.15-480.35 450.15-710.93	6 6 10 18	4 32 41 73	Boublik, T. et al Nasir, P. et al Stull, D. R. Wilson, G.M. et al	1973 1980 1947 1981	B A, Static C A, Static	16
10	C <sub>10</sub> H <sub>18</sub>	cis-Decalin	5.53-102.73 2.666-13.332 0.133-101.33 17.65-3571.48	373.033-469.526 353.65-397.65 295.65-467.75 406.21-727.59	19 5 10 17	4 1 41 73	Boublik, T. et al API 42 Stull, D. R. Wilson, G.M. et al	1973 1966 1947 1981	B A, C A, Static	

Table 4. Vapor pressure data on unsaturated ring compounds--Continued

No.	Formula	Name	Vapor Pressure Range, kPa	Temperature Range, K	Number of Data Points	Reference Number	Authors	Year Published	Data Types and Method of Measurement	Reference Citing the Same Data
11	C <sub>10</sub> H <sub>18</sub>	trans-Decalin	2.666-13.333 5.53-102.73 0.133-101.33	346.15-390.15 365.310-461.017 272.35-459.85	5 19 10	1 4 41	API 42 Boublik, T. et al Stull, D. R.	1966 1973 1947	A B C	
12	C <sub>11</sub> H <sub>14</sub>	1,1-Dimethylindan	0.258-101.325	313.15-467.22	24	37	Osborn, A.G. et al	1978	A, Ebullimetric	
13	C <sub>11</sub> H <sub>14</sub>	4,6-Dimethylindan	0.057-47.38	313.15-467.22	18	37	Osborn, A.G. et al	1978	A, Ebullimetric	
14	C <sub>11</sub> H <sub>14</sub>	4,7-Dimethylindan	0.050-47.375	313.15-469.97	17	37	Osborn, A.G. et al	1978	A, Ebullimetric	
15	C <sub>12</sub> H <sub>8</sub>	Biphenylene	0.0176-1.8352	338.15-408.15	16	56	Osborn, A.G. et al	1980	A, Static	
16	C <sub>12</sub> H <sub>10</sub>	Biphenyl	0.10-142.03 0.000416-363.57 0.58-880.0 0.000118-0.000123 2.04-400.11 0.016-0220 0.109-1108.576	342.35-544.25 288.20-595.45 373.2-653.2 297.15-297.85 396.14-600.69 326.2-354.2 343.15-673.15	15 75 13 15 12 4 16	4 6 17 22 32 40 72	Boublik, T. et al Coal Tar Res. Ass. Vargafik, N. B. Bradley, R.S. et al Nasir, F. et al Sharma, R.K. et al Chipman, J. et al	1973 1965 1975 1953 1980 1974 1929	B B B A, Effusion A, Static A, Chromatographic A, Isotenlescopic	
17	C <sub>12</sub> H <sub>16</sub>	Phenylcyclohexane	264.8-2457.3	560.93-727.59	7	73	Wilson, G.M. et al	1981	A, Static	
18	C <sub>12</sub> H <sub>22</sub>	Bicyclohexyl	9.59-346.69 0.067-1.333	424.25-577.25 321.15-376.15	23 5	44 1	Wiczorek, S.A. et al API 42	1980 1966	A, Static A	
19	C <sub>12</sub> H <sub>22</sub>	1,1-Dicyclo-pentylethane	0.067-1.333	385.65-430.65	5	1	API 42	1966	A,	
20	C <sub>13</sub> H <sub>12</sub>	Biphenylmethane	0.067-1.333 32.33-146.89 0.133-101.33 390-670.12 15.93-1827.1 0.032-38.565	343.2-400.2 490.69-555.39 349.15-537.65 424.64-647.25 560.93-727.59 313.15-468.64	5 9 10 32 7 18	1 16 41 44 73 37	API 42 Timmermans, J. Stull, D. R. Wiczorek, S.A. et al Wilson, G. M. et al Osborn, A. G. et al	1966 1965 1947 1980 1981 1978	A, B C A, Static A, Static A, Ebullimetric	
22	C <sub>13</sub> H <sub>18</sub>	1,1,4,7-Tetra-methylindan	0.025-31.177	313.15-468.80	18	37	Osborn, A. G. et al	1978	A, Ebullimetric	

Table 4. Vapor pressure data on unsaturated ring compounds---Continued

No.	Formula	Name	Vapor Pressure Range, kPa <sup>a</sup>	Temperature Range, K	Number of Data Points	Reference Number	Authors	Year Published	Data Types <sup>b</sup> and Method of Measurement	Reference Citing the Same Data
23	C <sub>14</sub> H <sub>12</sub>	Biphenylethylene	0.067-1.333	350.15-407.15	5	1	API 42	1966	A,	
24	C <sub>14</sub> H <sub>14</sub>	1,1-Diphenylethane	0.067-1.333	348.65-404.65	5	1	API 42	1966	A,	
25	C <sub>14</sub> H <sub>14</sub>	1,2-Diphenylethane	0.067-1.333 0.017-1.498	354.15-411.65 333.15-413.15	5 17	1 56	API 42 Osborn, A. G. et al	1966 1980	A, A, Static	
26	C <sub>14</sub> H <sub>20</sub>	2-Butyltetralin	0.067-1.333	354.65-410.65	5	1	API 42	1966	A,	
27	C <sub>14</sub> H <sub>20</sub>	1-Cyclohexyl-1-phenylethane	0.067-1.333	345.15-399.65	5	1	API 42	1966	A,	
28	C <sub>14</sub> H <sub>20</sub>	2-Cyclohexyl-1-phenylethane	0.067-1.333	348.15-406.15	5	1	API 42	1966	A,	
29	C <sub>14</sub> H <sub>20</sub>	3-Cyclopentyl-1-phenylpropane	0.067-1.333	348.15-406.15	5	1	API 42	1966	A,	
30	C <sub>14</sub> H <sub>26</sub>	1,1-Dicyclohexylethane	0.067-1.333	346.15-402.15	5	1	API 42	1966	A,	
31	C <sub>14</sub> H <sub>26</sub>	1,2-Dicyclohexylethane	0.067-1.333	347.65-402.15	5	1	API 42	1966	A,	

<sup>a</sup> 1 kPa = 7.50062 torr (mmHg)<sup>b</sup> A = Experimental Data Measured by the Author(s) of the Reference

B = Experimental Data collected from Literature by the Author(s) of the Reference

C = Calculated Values from a Regressed Correlation Based on Experimental Data

Table 5. Vapor pressure data on sulfur compounds

No.	Formula	Name	Vapor Pressure Range, kPa <sup>a</sup>	Temperature Range, K	Number of Data Points	Reference Number	Authors	Year Published	Data Types and Method of Measurement <sup>b</sup>	Reference Citing the Same Data
1	C <sub>2</sub> H <sub>4</sub> S	Thiacyclopropane	1.333-199.98 25.009-270.111	238.55-350.06 291.44-360.88	27 14	2 4	TRCHP Boublik, T. et al	1978 1973	C B	
2	C <sub>3</sub> H <sub>6</sub> S	Thiacyclobutane	1.333-199.98 19.920-270.111	268.25-392.68 321.507-404.789	27 15	2 36	TRCHP Osborn, A.G. et al	1978 1966	C A, Static 8 Ebulliometric	4, 15
3	C <sub>4</sub> H <sub>4</sub> S	Thiophene	1.333-199.98 19.920-270.111 0.00207-4543.6 0.107-119.99 44.93-172.52 0.133-101.33 482.6-5467.5	260.85-381.16 312.211-392.937 195.38-560.93 228.19-362.85 333.45-373.45 232.45-357.55 422.05-577.61	30 15 25 24 5 10 29	2 4 6 16 24 41 51	TRCHP Boublik, T. et al Coal Tar Res. Ass. Timmermans, J. Eon, C. et al Stull, D.R. Kobe, K. A. et al	1978 1973 1965 1965 1971 1947 1956	C B B B A, Isoteniscopic C A, Static	6, 15, 9 9 9 15
4	C <sub>4</sub> H <sub>8</sub> S	Tetrahydrothiophene	12.95-54.93	333.45-373.45	5	24	Eon, C. et al	1971	A, Isoteniscopic	15
5	C <sub>4</sub> H <sub>8</sub> S	Thiacyclopentane	1.333-199.98 1.333-199.98 19.920-270.111 11.67-122.51	287.35-420.609 287.38-420.61 344.332-433.601 331.31-401.56	27 27 15 19	2 2 36 43	TRCHP TRCHP Osborn, A.G. et al White, P.T. et al	1978 1978 1966 1952	C C A, Static & Ebulliometric A, Ebulliometric	15 4, 15, 16
6	C <sub>5</sub> H <sub>6</sub> S	2-Methylthiophene	1.333-199.98 17.20-71.33 0.133-101.33	282.15-411.15 333.45-373.45 245.75-385.65	30 5 10	2 24 41	TRCHP Eon, C. et al Stull, D. R.	1978 1971 1947	C A, Isoteniscopic C	15 9
7	C <sub>5</sub> H <sub>6</sub> S	3-Methylthiophene	1.333-199.98 15.47-65.33 0.133-101.33	284.15-414.15 333.45-373.45 248.65-388.55	30 5 10	2 24 41	TRCHP Eon, C. et al Stull, D.R.	1978 1971 1947	C A, Isoteniscopic C	15
8	C <sub>5</sub> H <sub>10</sub> S	Cyclopentanethiol	19.920-270.111	354.024-445.933	15	36	Osborn, A.G. et al	1966	A, State & Ebulliometric	4
9	C <sub>5</sub> H <sub>10</sub> S	2-Methylthiacyclopentane	1.333-199.98 9.582-270.111 11.64-116.28	295.87-432.811 335.783-446.240 340.94-411.49	27 21 18	2 36 43	TRCHP Osborn, A.G. et al White, P.T. et al	1978 1966 1952	C A, Static & Ebulliometric A, Ebulliometric	4, 15 9

Table 5. Vapor pressure data on sulfur compounds--Continued

No.	Formula	Name	Vapor Pressure Range, kPa <sup>a</sup>	Temperature Range, K	Number of Data Points	Reference Number	Authors	Year Published	Data Types <sup>b</sup> and Method of Measurement	Reference Citing the Same Data
10	C <sub>5</sub> H <sub>10</sub> S	3-Methylthiacyclopentane	1.333-199.98	300.25-439.026	27	2	TRCHP	1978	C	4,15 9
			9.582-270.111	340.690-452.626	21	36	Osborn, A.G. et al	1966	A, Static & Ebulliometric	
			11.68-133.03	345.71-422.38	20	43	White, P.T. et al	1952	A, Ebulliometric	
11	C <sub>5</sub> H <sub>10</sub> S	Thiacyclohexane	1.333-199.98	302.35-443.15	27	2	TRCHP	1978	C	15 9
			13.332-101.33	351.43-414.90	5	4	Boublik, T. et al	1973	B	
			11.65-129.10	348.01-422.16	17	43	White, P.T. et al	1952	A, Ebulliometric	
12	C <sub>6</sub> H <sub>10</sub> S	Benzenethiol	1.333-199.98	325.43-471.102	27	2	TRCHP	1978	C	4,15 9
			19.920-270.111	387.693-485.310	15	36	Osborn, A.G. et al	1966	A, Static & Ebulliometric	
			0.133-101.33	291.75-441.15	10	41	Stull, D.R.	1947	C	
13	C <sub>6</sub> H <sub>8</sub> S	2,5-Dimethylthiophene	2.000-101.33	339.15-441.15	9	9	Haines, W.E. et al	1963	B	4,15 9
			7.40-34.26	333.45-373.45	5	24	Eon, C. et al	1971	A, Isoteniscopic	
14	C <sub>6</sub> H <sub>8</sub> S	2-Ethylthiophene	8.12-37.33	333.45-373.45	5	24	Eon, C. et al	1971	A, Isoteniscopic	
15	C <sub>6</sub> H <sub>12</sub> S	Cyclohexanthiol	9.582-270.111	356.89-475.80	21	36	Osborn, A.G. et al	1966	A, Static & Ebulliometric	4,15 9
			1.60-101.32	314.15-431.15	6	9	Haines, W.E. et al	1963	B	
16	C <sub>6</sub> H <sub>12</sub> S	2-cis-5-Dimethylthiacyclopentane	1.333-199.98	303.15-444.15	27	2	TRCHP	1978	C	9
			11.65-133.01	348.86-426.37	19	43	White, P.T. et al	1952	A, Ebulliometric	
17	C <sub>6</sub> H <sub>12</sub> S	2-trans-5-Dimethylthiacyclopentane	1.333-199.98	302.15-443.15	27	2	TRCHP	1978	C	9
			11.65-59.39	348.05-395.82	13	43	White, P.T. et al	1952	A, Ebulliometric	
18	C <sub>6</sub> H <sub>12</sub> S	2-Methylthiacyclohexane	1.333-199.98	309.15-455.15	30	2	TRCHP	1978	C	9
			11.65-133.10	356.84-437.32	20	43	White, P.T. et al	1952	A, Ebulliometric	
19	C <sub>6</sub> H <sub>12</sub> S	3-Methylthiacyclohexane	1.333-199.98	313.15-460.15	30	2	TRCHP	1978	C	9
			11.65-91.59	361.23-427.18	15	43	White P.T. et al	1952	A, Ebulliometric	
20	C <sub>6</sub> H <sub>12</sub> S	4-Methylthiacyclohexane	1.333-199.98	314.15-461.15	30	2	TRCHP	1978	C	9
			11.65-122.01	361.66-439.37	19	43	White, P.T. et al	1952	A, Ebulliometric	

Table 5. Vapor pressure data on sulfur compounds--Continued

No.	Formula	Name	Vapor Pressure Range, kPa <sup>a</sup>	Temperature Range, K	Number of Data Points	Reference Number	Authors	Year Published	Data Types and Method of Measurement	Reference Citing the Same Data
21	C <sub>7</sub> H <sub>8</sub> S	2-Methylbenzenethiol	1.333-199.98	343.15-498.15	27	2	TRCHP	1978	C	
22	C <sub>7</sub> H <sub>8</sub> S	3-Methylbenzenethiol	1.333-199.98	345.15-498.15	27	2	TRCHP	1978	C	
23	C <sub>7</sub> H <sub>8</sub> S	4-Methylbenzenethiol	1.333-199.98	343.15-499.15	27	2	TRCHP	1978	C	
24	C <sub>7</sub> H <sub>8</sub> S	1-Thiaethylbenzene	9.582-120.798 0.800-98.26	390.296-474.772 332.2-467.2	16 10	36 9	Osborn, A.G. et al Haines, V.E. et al	1966 1963	A, Static & B	Ebulliometric. 4
25	C <sub>10</sub> H <sub>8</sub> S	1-Naphthalenethiol	0.200-101.33	379.15-559.15	8	9	Haines, V.E. et al	1963	B	
26	C <sub>10</sub> H <sub>8</sub> S	2-Naphthalenethiol	1.373-101.33	419.45-559.15	6	9	Haines, V.E. et al	1963	B	
27	C <sub>12</sub> H <sub>8</sub> S	Dibenzothiophene	0.471-105.902	424.81-607.53	19	75	Sivaraman, A. et al	1982	A, Static	
28	C <sub>12</sub> H <sub>8</sub> S	Diphenylthiomethane	0.00267-101.33	368.2-569.2	17	9	Haines, V.E. et al	1963	B	

<sup>a</sup> 1 kPa = 7.50062 torr (mmHg)<sup>b</sup> A = Experimental Data Measured by the Author(s) of the Reference

B = Experimental Data Collected from Literature by the Author(s) of the Reference

C = Calculated Values from a Regressed Correlation Based on Experimental Data





Table 6. Vapor pressure data on nitrogen compounds-I--Continued

No.	Formula	Name	Vapor Pressure Range, kPa <sup>a</sup>	Temperature Range, K	Number of Data Points	Reference	Authors	Year Published	Data Types, Methods of Measurement <sup>b</sup>	Reference Citing the Same Data Set
38	C <sub>9</sub> H <sub>7</sub> N	Isoquinoline	13.412-102.29	439.93-516.85	40	4	Boublik, T., et al.	1973	B	15
			0.807-101.33	373.9-513.3	14	6	Coal Tar Res. Ass.	1965	B	
			0.009-4479.0	300.-780.	201	8	Eng. Sci. Data Unit	1978	C	
			0.133-101.3	336.7-513.7	10	41	Stull, D.R.	1947	C	
39	C <sub>9</sub> H <sub>7</sub> N	Quinoline	15.997-102.02	437.82-511.09	28	4	Boublik, T., et al.	1973	B	15
			0.340-101.3	348.5-510.7	24	6	Coal Tar Res. Ass.	1965	B	
			0.001-3731.5	265.-780.	204	8	Eng. Sci. Data Unit	1978	C	
			0.340-99.37	348.5-509.80	69	16	Timmermans, J.	1965	B	
			0.00385-0.0243	285.77-309.05	8	42	van De Rosstyn, C., et al.	1980	A, Gas-saturation	
			164.1-2806.2	533.15-727.59	8	73	Wilson, G. M., et al.	1981	A, Static	
40	C <sub>8</sub> H <sub>9</sub> N	4-Cumidine	0.133-101.3	332.9-510.9	10	41	Stull, D.R.	1947	C	10
			0.133-101.3	333.15-500.15	10	41	Stull, D.R.	1947	C	
41	C <sub>8</sub> H <sub>9</sub> N	4-Isopropylaniline	0.003-3238.6	280.-715.	88	8	Eng. Sci. Data Unit	1978	C	
42	C <sub>8</sub> H <sub>9</sub> N	N,N,2-Trimethylaniline	0.001-3223.7	245.-665.	85	8	Eng. Sci. Data Unit	1978	C	
			0.667-13.33	439.3-391.3	47	16	Timmermans, J.	1965	B	
43	C <sub>9</sub> H <sub>9</sub> N	N,N,4-Trimethylaniline	0.001-3750.0	265.-695.	87	8	Eng. Sci. Data Unit	1978	C	
			0.133-101.3	323.3-482.7	10	41	Stull, D.R.	1947	C	
44	C <sub>9</sub> H <sub>9</sub> N	2,4,5-Trimethylaniline	0.154-3500.0	340.-725.	78	8	Eng. Sci. Data Unit	1978	C	
			0.133-101.33	341.6-507.7	10	41	Stull, D.R.	1947	C	
45	C <sub>10</sub> H <sub>9</sub> N	3-Methylisoquinoline	12.27-104.66	449.46-527.74	25	4	Boublik, T., et al.	1973	B	15
			0.001-4856.9	285.-780.	205	8	Eng. Sci. Data Unit	1978	C	
46	C <sub>10</sub> H <sub>9</sub> N	2-Methylquinoline	0.001-4800.8	280.-785.	202	8	Eng. Sci. Data Unit	1978	C	10, 15
			0.133-101.33	348.45-519.65	10	41	Stull, D.R.	1947	C	
47	C <sub>10</sub> H <sub>9</sub> N	4-Methylquinoline	0.001-4554.4	295.-795.	201	8	Eng. Sci. Data Unit	1978	C	
			16.719-101.75	471.73-538.97	22	4	Boublik, T., et al.	1973	B	
48	C <sub>10</sub> H <sub>9</sub> N	6-Methylquinoline	12.113-101.71	459.64-539.29	26	4	Boublik, T., et al.	1973	B	15
			0.001-3628.2	290.-795.	202	8	Eng. Sci. Data Unit	1978	C	
49	C <sub>10</sub> H <sub>9</sub> N	7-Methylquinoline	63.168-101.90	511.-531.15	17	4	Boublik, T., et al.	1973	B	15
			0.001-4854.7	290.-790.	201	8	Eng. Sci. Data Unit	1978	C	
50	C <sub>10</sub> H <sub>9</sub> N	8-Methylquinoline	61.222-101.87	500.46-521.30	15	4	Boublik, T., et al.	1973	B	15
			0.001-4950.8	280.-790.	203	8	Eng. Sci. Data Unit	1978	C	
51	C <sub>10</sub> H <sub>9</sub> N	1-Naphthylamine	0.005-385.56	325.-645.	65	8	Eng. Sci. Data Unit	1978	C	
			0.161-351.60	385.-645.	53	8	Eng. Sci. Data Unit	1978	C	
53	C <sub>10</sub> H <sub>9</sub> N	Quinaldine	15.225-101.62	451.45-521.01	41	4	Boublik, T., et al.	1973	B	
			0.00143-0.0180	281.90-312.64	9	42	van De Rosstyn, C., et al.	1980	A, Gas-saturation	
54	C <sub>10</sub> H <sub>9</sub> N	N,N-Diethylaniline	0.001-3684.2	265.-785.	77	8	Eng. Sci. Data Unit	1978	C	15
			0.133-101.33	322.9-488.7	10	41	Stull, D.R.	1947	C	
55	C <sub>11</sub> H <sub>11</sub> N	2,4-Dimethylquinoline	0.213-106.6	323.2-491.55	30	66	Nelson, O.A., et al.	1925	A, Isoteniscope	15
			11.79-106.53	458.5-542.60	19	4	Boublik, T., et al.	1973	B	
56	C <sub>11</sub> H <sub>11</sub> N	2,6-Dimethylquinoline	0.001-3826.2	295.-785.	203	8	Eng. Sci. Data Unit	1978	C	15
			13.416-100.66	461.61-539.44	27	4	Boublik, T., et al.	1973	B	
57	C <sub>11</sub> H <sub>11</sub> N	Carbazol	0.001-3753.3	290.-780.	203	8	Eng. Sci. Data Unit	1978	C	10, 15
			9.346-107.62	525.76-630.86	34	4	Boublik, T., et al.	1973	B	
58	C <sub>12</sub> H <sub>11</sub> N	Diphenylamine	7.33-99.19	518.0-625.2	18	6	Coal Tar Res. Ass.	1965	B	
			0.003-555.48	330.-670.	69	8	Eng. Sci. Data Unit	1978	C	
59	C <sub>13</sub> H <sub>9</sub> N	Acridine	60.90-72.26	551.-558.	8	16	Timmermans, J.	1965	B	10
			0.133-101.33	381.45-575.15	10	41	Stull, D.R.	1947	C	
60	C <sub>13</sub> H <sub>9</sub> N	N-Methyldiphenylamine	0.65810-1.0710	281.11-323.15	11	29	McEwen, D.M., et al.	1975	A	6, 10, 15
			0.133-101.33	402.6-519.2	10	41	Stull, D.R.	1947	C	
61	C <sub>14</sub> H <sub>13</sub> N	N-Ethylcarbazol	0.00247-0.0147	347.81-373.80	7	42	van De Rosstyn, C., et al.	1980	A, Gas-saturation	
			0.001-583.05	310.-670.	73	8	Eng. Sci. Data Unit	1978	C	
62	C <sub>14</sub> H <sub>13</sub> N	N-Ethyldiphenylamine	0.001-482.57	320.-670.	71	8	Eng. Sci. Data Unit	1978	C	
			0.133-101.33	391.5-573.2	10	41	Stull, D.R.	1947	C	
64	C <sub>19</sub> H <sub>17</sub> N	N-Methyldiphenylaniline	0.001-623.62	310.-670.	73	8	Eng. Sci. Data Unit	1978	C	
			0.001-623.62	310.-670.	73	8	Eng. Sci. Data Unit	1978	C	

<sup>a</sup> 1 kPa = 7.50062 torr (mm Hg).

<sup>b</sup> A = experimental data measured by the author(s) of the reference.  
 B = experimental data collected from literature by the author(s) of the reference.  
 C = calculated values from a regressed correlation based on experimental data.

<sup>c</sup> Ebull. = Ebulliometric

Table 7. Vapor pressure data on nitrogen compounds-II

No.	Formula	Name	Vapor Pressure Range, kPa <sup>a</sup>	Temperature Range, K	Number of Data Points	Reference	Authors	Year Published	Data Types <sup>b</sup> , Methods of Measurement
1	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub>	Pyrazine	12.755-5673.0	330.-620.	59	8	Eng. Sci. Data Unit	1978	C
2	C <sub>4</sub> H <sub>10</sub> N <sub>2</sub>	Piperazine	0.165-4553.3	270.-655.	61	8	Eng. Sci. Data Unit	1978	C
3	C <sub>5</sub> H <sub>6</sub> N <sub>2</sub>	2-Methylpyrazine	2.392-4777.6	310.-630.	65	8	Eng. Sci. Data Unit	1978	C
4	C <sub>5</sub> H <sub>12</sub> N <sub>2</sub>	1-Methylpiperazine	0.001-4550.0	230.-630.	81	8	Eng. Sci. Data Unit	1978	C
5	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub>	1,3-Diaminobenzene	0.012-1587.7	340.-720	77	8	Eng. Sci. Data Unit	1978	C
6	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub>	1,3-Phenylenediamine	0.133-101.33	373.0-558.7	10	41	Stull, D.R.	1947	C
7	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub>	Phenyldiazine	0.133-101.33	345.-7491.4	10	41	Stull, D.R.	1947	C
8	C <sub>6</sub> H <sub>14</sub> N <sub>2</sub>	cis-2,5-Dimethylpiperazine	0.137-12.00	373.-465.	70	8	Williams, G.E., et al.	1942	Asc, Isoteniscopic
9	C <sub>7</sub> H <sub>10</sub> N <sub>2</sub>	4-Amino-2,6-dimethylpyridine	0.103-3000.0	290.-635.	70	8	Eng. Sci. Data Unit	1978	C
10	C <sub>7</sub> H <sub>10</sub> N <sub>2</sub>	2,4-Diaminotoluene	20.251-3820.7	460.-745.	58	8	Eng. Sci. Data Unit	1978	C
11	C <sub>8</sub> H <sub>18</sub> N <sub>2</sub>	Tetramethylpiperazine	0.091-1440.6	375.-720.	70	8	Eng. Sci. Data Unit	1978	C
12	C <sub>10</sub> H <sub>14</sub> N <sub>2</sub>	1-Phenylpiperazine	0.001-2488.2	295.-645.	71	8	Eng. Sci. Data Unit	1978	C
13	C <sub>12</sub> H <sub>8</sub> N <sub>2</sub>	Phenazine	0.133-101.33	286.9-456.7	10	41	Stull, D.R.	1947	C
14	C <sub>12</sub> H <sub>10</sub> N <sub>2</sub>	Azobenzene	0.001-561.33	300.-655.	72	8	Eng. Sci. Data Unit	1978	C
15	C <sub>13</sub> H <sub>14</sub> N <sub>2</sub>	Di-(4-aminophenyl)-methane	0.48x10 <sup>-6</sup> -6.23x10 <sup>-5</sup>	281.11-323.15	12	29	McEachern, D.M., et al.	1975	A (solid)
16	C <sub>3</sub> H <sub>3</sub> NO	Isoxazole	0.133-101.33	376.7-566.2	10	41	Stull, D.R.	1947	C
17	C <sub>3</sub> H <sub>3</sub> NO	Oxazole	0.001-325.17	375.-720.	70	8	Eng. Sci. Data Unit	1978	C
18	C <sub>6</sub> H <sub>5</sub> NO <sub>3</sub>	2-Nitrophenol	0.001-3741.8	195.-550.	72	8	Eng. Sci. Data Unit	1978	C
			0.001-3629.1	180.-510.	67	8	Eng. Sci. Data Unit	1978	C
			0.133-101.33	322.5-487.7	10	41	Stull, D.R.	1947	C

<sup>a</sup> 1 kPa = 7.50062 torr (mm Hg)

<sup>b</sup> A = experimental data measured by the author(s) of the reference.  
 B = experimental data collected from literature by the author(s) of the reference.  
 C = calculated values from a regressed correlation based on experimental data.

Table 8. Vapor pressure data on oxygen compounds-I

No.	Formula	Name	Vapor Pressure Range, kPa <sup>a</sup>	Temperature Range, K	Number of Data Points	Reference Numbers	Author(s)	Year Published	Data Types and Method of Measurement <sup>b</sup>	Reference Citing the Same Data
1	C <sub>4</sub> H <sub>4</sub> O	Furan	31.167276.11	275.702-334.590	13	4	Boublik, T., et al.	1973	B	
			0.0027500.	193.157-480.25	27	14	Kudchadker, A.P., et al.	1978	B	
			627.4*5012.5	366.50*483.17	22	51	Kobe, K.A., et al.	1956	A, Static	15
2	C <sub>6</sub> H <sub>8</sub> O	Cyclobutanone	0.2675.760	249.097-298.39	11	4	Boublik, T., et al.	1973	B	
			19.9270.11	296.289-372.850	15	4	Boublik, T., et al.	1973	B	
			1.9545190.	253.15*540.15	25	14	Kudchadker, A.P., et al.	1978	C	
3	C <sub>6</sub> H <sub>8</sub> O	Tetrahydrofuran	434.4*5053.8	394.28*538.72	27	51	Kobe, K.A., et al.	1956	A, Static	15
			86.13*283.98	333.45*373.45	5	24	Ion, C., et al.	1971	A, Isotenisometric	
			358.5*4722.9	303.17*527.61	27	51	Kobe, K.A., et al.	1956	A, Static	15
4	C <sub>6</sub> H <sub>8</sub> O	2-Methylfuran	0.3071.600	273.097-296.79	4	4	Boublik, T., et al.	1973	B	
			634.3*3557.8	427.61*533.17	20	51	Kobe, K.A., et al.	1956	A, Static	15
			1.333199.98	345.72*481.57	27	2	TRCP	1978	C	
5	C <sub>6</sub> H <sub>8</sub> O	Cyclopentanone	7.6057101.33	380.30*454.90	6	4	Boublik, T., et al.	1973	B	
			0.00373*102.27	273.15*455.33	33	6	Coal Tar Res. Ass.	1965	B	10
			0.0104*6130.	283.2*694.25	29	11	Kudchadker, A.P., et al.	1978	C	
6	C <sub>6</sub> H <sub>8</sub> O	2-Methyl tetrahydrofuran	0.006675.666	278.55*377.85	79	16	Timmenmans, J.	1965	B	
			0.31*59271.	340.85*631.15	20	18	Jaw, C.	1978	C	
			0.133*6078	313.25*691.85	19	41	Stull, D.R.	1947	C	10
7	C <sub>6</sub> H <sub>8</sub> O	Phenol	12.725*131.422	362.78*438.92	16	31	Meyer, E.F., et al.	1973	A, Bullionometric	15
			0.133*101.33	274.55*428.75	10	41	Stull, D.R.	1947	C	
			0.133*101.33	294.15*434.15	10	41	Stull, D.R.	1947	C	
8	C <sub>6</sub> H <sub>10</sub> O	Cyclohexanone	7.843*99.192	366.88*433.85	16	15	Shum, O.	1976	B	
			0.133*101.33	280.85*400.65	10	41	Stull, D.R.	1947	C	
			449.95*342.85	369.15*522.35	10	41	Stull, D.R.	1947	C	
9	C <sub>6</sub> H <sub>10</sub> O	Cyclohexanol	6.287*67.661	346.49*412.52	6	16	Timmenmans, J.	1965	B	
			0.133*101.33	334.05*463.65	19	2	TRCP	1978	C	
			1.333199.98	350.10*492.06	49	4	TRCP	1978	C	
10	C <sub>6</sub> H <sub>10</sub> O	2-Hexanone	10.11*101.33	393.37*464.10	5	4	Boublik, T., et al.	1973	B	
			0.00267*104.98	273.15*465.51	26	6	Coal Tar Res. Ass.	1965	B	10, 15
			0.007479*5010.	283.2*697.65	28	12	Kudchadker, A.P., et al.	1978	C	
11	C <sub>6</sub> H <sub>10</sub> O	3-Hydroxytoluene	0.133*101.33	309.75*383.45	49	16	Timmenmans, J.	1965	B	
			0.133*101.33	311.35*463.95	10	41	Stull, D.R.	1947	C	10
			1.333199.98	360.90*503.17	27	2	TRCP	1978	C	
12	C <sub>6</sub> H <sub>10</sub> O	4-Hydroxytoluene (4-Cresol)	20.27*98.93	422.65*474.25	12	4	Boublik, T., et al.	1973	B	
			0.00231*105.53	273.15*476.93	26	6	Coal Tar Res. Ass.	1965	B	10, 15
			0.007479*4560.	283.2*705.85	29	12	Kudchadker, A.P., et al.	1978	C	
13	C <sub>6</sub> H <sub>10</sub> O	Methoxybenzene (Anisole)	4.119*1124.29	388.12*595.63	15	32	Nasir, P., et al.	1980	A, Static	
			0.133*101.33	325.15*475.95	10	41	Stull, D.R.	1947	C	10
			1.333199.98	361.45*502.78	27	2	TRCP	1978	C	
14	C <sub>6</sub> H <sub>10</sub> O	2-Hydroxytoluene (2-Cresol)	8.85*101.33	401.20*475.03	6	4	Boublik, T., et al.	1973	B	
			0.00147*104.13	273.15*476.14	24	6	Coal Tar Res. Ass.	1965	B	10, 15
			0.00322*5150	283.2*704.65	29	12	Kudchadker, A.P., et al.	1978	C	
15	C <sub>6</sub> H <sub>10</sub> O	3-Hydroxytoluene	0.133*101.33	328.85*394.45	50	16	Timmenmans, J.	1965	B, Static	
			0.133*101.33	326.15*474.95	10	41	Stull, D.R.	1947	C	10
			0.0107*0.1640	273.15*313.15	7	6	Coal Tar Res. Ass.	1965	B	
16	C <sub>6</sub> H <sub>10</sub> O	4-Hydroxytoluene (4-Cresol)	1.373*3.253	352.65*370.85	9	16	Timmenmans, J.	1965	B	
			0.133*101.33	310.45*475.15	19	41	Stull, D.R.	1947	C	10
			1.333199.98	350.15*480.65	19	4	Boublik, T., et al.	1973	B	6
17	C <sub>6</sub> H <sub>10</sub> O	2-Ethylphenol	0.133*101.33	319.35*480.65	10	41	Stull, D.R.	1947	C	10
			0.00335*141.030	278.17*491.197	28	15	Shum, O.	1976	B	6
			1.333199.98	370.47*502.297	19	2	TRCP	1978	C	
18	C <sub>6</sub> H <sub>10</sub> O	3-Ethylphenol	0.133*101.33	333.15*487.15	10	41	Stull, D.R.	1947	C	10
			0.000947*133.414	278.11*502.742	27	15	Shum, O.	1976	B	6
			1.333199.98	374.15*491.35	19	4	Boublik, T., et al.	1973	B	6
19	C <sub>6</sub> H <sub>10</sub> O	4-Ethylphenol	0.000480*133.418	278.15*502.297	26	15	Shum, O.	1976	B	6
			1.333199.98	369.68*519.55	27	2	TRCP	1978	C	
			0.133*105.40	357.150*491.617	41	4	Boublik, T., et al.	1973	B	
20	C <sub>6</sub> H <sub>10</sub> O	2,3-Dimethylphenol	0.00029*49957.	278.2*722.95	25	13	Kudchadker, A.P., et al.,	1978	C	
			0.133*101.33	329.1*491.15	10	41	Stull, D.R.	1947	C	10
			0.00061*105.40	283.06*491.62	29	58	Andon, R.J.L., et al.	1960	A, Bullionometric	6, 15
21	C <sub>6</sub> H <sub>10</sub> O	2,4-Dimethylphenol	1.333199.98	366.02*513.04	27	2	TRCP	1978	C	
			0.00308*4400.	278.2*722.95	25	13	Kudchadker, A.P., et al.	1978	C	
			0.133*101.33	324.95*484.65	10	41	Stull, D.R.	1947	C	10
22	C <sub>6</sub> H <sub>10</sub> O	2,5-Dimethylphenol	0.00304*104.93	282.88*485.47	30	58	Andon, R.J.L., et al.	1960	A, Bullionometric	4, 6, 10, 15
			24.34*5005.28	431.87*727.59	19	73	Wilson, G.N., et al.	1961	A, Static	
			1.333199.98	365.69*513.39	27	2	TRCP	1978	C	
23	C <sub>6</sub> H <sub>10</sub> O	2,6-Dimethylphenol	0.00038*4900.	278.2*707.05	29	13	Kudchadker, A.P., et al.	1978	C	
			0.133*101.33	324.95*484.65	10	41	Stull, D.R.	1947	C	10
			0.00060*102.87	282.58*484.89	10	41	Stull, D.R.	1947	C	10
24	C <sub>6</sub> H <sub>10</sub> O	3,4-Dimethylphenol	1.333199.98	369.68*519.55	27	2	TRCP	1978	C	
			0.00267*4300.	278.2*701.05	29	13	Kudchadker, A.P., et al.	1978	C	
			0.00260*107.738	277.90*476.68	29	58	Andon, R.J.L., et al.	1960	A, Bullionometric	4, 6, 15
25	C <sub>6</sub> H <sub>10</sub> O	3,5-Dimethylphenol	1.333199.98	369.68*519.55	27	2	TRCP	1978	C	
			0.000155*9000.	278.2*729.95	29	13	Kudchadker, A.P., et al.	1978	C	
			0.133*101.33	339.35*496.35	10	41	Stull, D.R.	1947	C	10
26	C <sub>6</sub> H <sub>10</sub> O	3,4-Dimethylphenol	0.00029*106.371	283.04*502.05	30	58	Andon, R.J.L., et al.	1960	A, Bullionometric	4, 6, 15
			1.333199.98	376.55*523.67	27	2	TRCP	1978	C	
			0.000242*3600.	278.2*715.65	28	13	Kudchadker, A.P., et al.	1978	C	
27	C <sub>6</sub> H <sub>10</sub> O	3,5-Dimethylphenol	0.133*101.33	335.15*492.65	10	41	Stull, D.R.	1947	C	10
			0.00044*105.575	282.72*496.474	31	58	Andon, R.J.L., et al.	1960	A, Bullionometric	4, 6, 15
			0.133*101.33	393.65*523.67	27	2	TRCP	1978	C	
28	C <sub>6</sub> H <sub>10</sub> O	5-Indanol	0.133*101.33	382.85*460.25	10	41	Stull, D.R.	1947	C	
			0.133*101.33	306.85*469.65	10	41	Stull, D.R.	1947	C	
			0.133*101.33	306.85*469.65	10	41	Stull, D.R.	1947	C	
29	C <sub>6</sub> H <sub>10</sub> O	2-Ethylanisole	0.133*101.33	306.85*469.65	10	41	Stull, D.R.	1947	C	
			1.333199.98	384.65*506.15	19	4	Boublik, T., et al.	1973	B	6, 15
			1.333199.98	369.85*487.65	19	4	Boublik, T., et al.	1973	B	10, 15
30	C <sub>6</sub> H <sub>10</sub> O	3-Ethylanisole	0.133*101.33	329.75*487.65	10	41	Stull, D.R.	1947	C	10, 15
			1.333199.98	335.15*501.35	19	41	Stull, D.R.	1947	C	10, 15
			1.333199.98	381.35*501.35	19	4	Boublik, T., et al.	1973	B	10, 15
31	C <sub>6</sub> H <sub>10</sub> O	4-Ethylanisole	0.133*101.33	347.85*506.15	10	41	Stull, D.R.	1947	C	15
			1.333199.98	377.45*494.65	19	4	Boublik, T., et al.	1973	B	15
			3.333101.33	392.15*507.65	18	4	Boublik, T., et al.	1973	B	15
32	C <sub>6</sub> H <sub>10</sub> O	3-Methyl-5-ethylphenol	26.547*133.34	459.632*520.212	17	4	Boublik, T., et al.	1973	B	15
			1.333199.98	414.65*555.65	19	4	Boublik, T., et al.	1973	B	6, 15
			0.133*101.33	367.15*555.65	19	41	Stull, D.R.	1947	C	
33	C <sub>6</sub> H <sub>10</sub> O	2-Isopropylphenol	0.667*101.33	401.75*561.15	9	41	Stull, D.R.	1947	C	6, 15
			0.133*101.33	345.25*510.15	10	41	Stull, D.R.	1947	C	15
			26.543*133.40	451.885*512.662	17	4	Boublik, T., et al.	1973	B	15
34	C <sub>6</sub> H <sub>10</sub> O	4-Isopropylphenol	0.133*101.33	330.55*501.15	10	41	Stull, D.R.	1947	C	15
			0.133*101.33	340.15*501.35	10	41	Stull, D.R.	1947	C	15
			0.133*101.33	347.85*506.15	10	41	Stull, D.R.	1947	C	15
35	C <sub>6</sub> H <sub>10</sub> O	3-Phenyl-1-propanol	1.333199.98	377.45*494.65	19	4	Boublik, T., et al.	1973	B	15
			0.133*101.33	377.45*494.65	19	4	Boublik, T., et al.	1973	B	15
			3.333101.33	392.15*507.65	18	4	Boublik, T., et al.	1973	B	15
36	C <sub>6</sub> H <sub>10</sub> O	2-Propylphenol	26.547*133.34	459.632*520.212	17	4	Boublik, T., et al.	1973	B	15
			1.333199.98	414.65*555.65	19	4	Boublik, T., et al.	1973	B	6, 15
			0.133*101.33	367.15*555.65	19	41	Stull, D.R.	1947	C	

4. Results and Discussion

The most reliable vapor pressure data points were adopted for fitting into a Cox equation for each selected compound. The equation which yielded the least deviation of the calculated vapor pressures from the experimental values by a least-squares fit was accepted to represent the vapor pressure of the given compound.

The coefficients of the Cox equations for the seven classes of compounds are presented in Tables 10-18. Also included in each table are compound number, compound name, vapor pressure range (kPa) and temperature range (K) covered, calculated vapor pressure at 400 K, absolute average deviation (AAD), number of data points, and the reference numbers for the vapor pressure data used in the fit that yielded the listed coefficients.

As indicated in the tables, there are many cases where more than 100 data points were employed for fitting into a Cox equation for one compound. The average value of AAD for benzene and its derivatives is 0.37% which is excellent. The corresponding value for sulfur and nitrogen compounds is 0.39% and 0.45%, respectively. This value is higher for the other classes of compounds, probably due to the poor quality of the vapor pressure data employed for fitting.

The Cox equation can be used to fit a wide range of vapor pressures with reasonable precision (see Tables 10, 15, and 16). Using the listed coefficients of the Cox equation, we calculated the vapor pressure at 400 K for each compound as examples.

The vapor pressures of benzene were listed in TRC Hydrocarbon Project Tables as k, kb, and k-E Tables. The k table covered the temperature range from 263.74 to 377 K; while the kb table covered 368.15-543.15 K. The k-E table presented the vapor pressures of benzene (in lb in.<sup>-2</sup>) in the temperature range from 10-220 °F.<sup>2</sup> The vapor pressures in the k table were represented by an Antoine equation. Those in the kb table were represented by a modified Antoine equation.

A consistent set of vapor pressures for benzene was reported by Ambrose *et al.*<sup>33,35</sup> and was fitted to a Chebyshev polynomial.<sup>8</sup> However, it is not convenient to obtain  $dP/dT$  from the Chebyshev polynomial vapor pressure equation for calculating enthalpy of vaporization ( $\Delta H_v$ ) using the Clapeyron equation.

Based upon the Cox equation, the values of  $dP/dT$  and  $-[d(\ln P)/d(1/T)]$  may be obtained as follows<sup>79</sup>:

$$\frac{dP}{dT} = 2.303P \left[ \frac{D}{T^2} + \left(1 - \frac{D}{T}\right) (2.303B + 4.606CT) \right] \times \exp[2.303(A + BT + CT^2)],$$

and

$$-\frac{d(\ln P)}{d(1/T)} = 2.303 \left[ D + \left(1 - \frac{D}{T}\right) (2.303BT^2 + 4.606CT^3) \right] \times \exp[2.303(A + BT + CT^2)],$$

where the quantities  $A, B, C,$  and  $D$  are known from the Cox equation.

TABLE 9. Vapor Pressure Data on More Oxygen Compounds - II

No.	Formula	Name	Vapor Pressure Range, kPa <sup>a</sup>	Temperature Range, K	Number of Data Points	Reference Number	Author(s)	Year Published	Data Types and Method of Measurement <sup>b</sup>	Reference Citing the same Data
1	C <sub>6</sub> H <sub>4</sub> O <sub>2</sub>	Quinone (p-Benzoquinone)	0.280-2.027	259.85-278.45	4	16	Timmermans, J.	1965	B	
2	C <sub>6</sub> H <sub>6</sub> O <sub>2</sub>	1,2-Dihydroxybenzene (Pyrocatechol)	1.333-101.33	391.65-518.65	19	4	Boublik, T., et al.	1973	B	
3	C <sub>6</sub> H <sub>6</sub> O <sub>2</sub>	1,3-Dihydroxybenzene (Resorcinol)	0.133-101.33	377.15-518.65	10	41	Sculi, D.R.	1947	C	
4	C <sub>6</sub> H <sub>6</sub> O <sub>2</sub>	1,4-Dihydroxybenzene (Hydroquinone)	0.133-101.33	424.65-549.65	19	4	Boublik, T., et al.	1973	B	6
5	C <sub>6</sub> H <sub>6</sub> O <sub>3</sub>	Pyrogallol	0.133-101.33	381.55-549.65	19	4	Sculi, D.R.	1947	B	
6	C <sub>7</sub> H <sub>8</sub> O	Quilicool	0.133-101.33	432.25-559.15	19	16	Boublik, T., et al.	1973	B	6
7	C <sub>12</sub> H <sub>6</sub> O	Diphenylene Oxide	0.133-101.33	428.15-541.05	14	4	Timmermans, J.	1965	C	
8	C <sub>12</sub> H <sub>6</sub> O	Dibenzofuran	0.626-171.714	405.55-559.35	10	41	Sculi, D.R.	1947	C	
9	C <sub>12</sub> H <sub>10</sub> O <sub>2</sub>	2,2-Diphenol	5.186-291.677	450.45-582.15	19	4	Boublik, T., et al.	1973	B	
10	C <sub>12</sub> H <sub>10</sub> O <sub>4</sub>	Quinhydrone	1.333-101.33	424.85-582.15	19	41	Sculi, D.R.	1947	C	
11	C <sub>14</sub> H <sub>8</sub> O <sub>4</sub>	Antharthrone	0.004346-107.285	355.15-478.15	19	4	Boublik, T., et al.	1973	B	
				377.01-586.46	6	74	Coal Tar Res. Ass.	1965	B	
				435.35-618.05	19	75	Nasir, P., et al.	1982	A, Static	
				444.15-598.15	19	4	Sivaraman, A., et al.	1982	A, Static	15
				317.55-333.55	6	16	Boublik, T., et al.	1973	B	
				558.73-656.33	33	10	Timmermans, J. Jordan, T.E.	1965 1954	B C	

<sup>a</sup> 1 kPa = 7.50062 torr (mm Hg)

<sup>b</sup> A = Experimental data measured by the author(s) of the reference.  
B = Experimental data collected from literature by the author(s) of the reference.

C = Calculated values from a regressed correlation based on experimental data.

TABLE 10. Coefficients of vapor pressure equation and the calculated vapor pressures at 400 K for benzene and its derivatives

No.	Name	$\log_{10} P = (A - D/T) \times 10 + (B + CT + CT^2) \times 10^{-4}$				Vapor Pressure Range, kPa	Temperature Range, K	Calculated Vapor Pressure at 400.0 K, kPa	AAD <sup>b</sup> , %	Number of Data	Data Reference Numbers
		A	B x 10 <sup>4</sup>	C x 10 <sup>7</sup>	D						
1	Benzene	0.832632	-6.72598	6.38324	353.214	5.13 - 4924.0	280.0 <sup>c</sup> -562.6	352.73	131	8, 17, 24, 35, 55	
2	Toluene	0.837122	-6.48791	5.91293	383.737	0.919 - 4016.3	245.0 <sup>c</sup> -590.0	157.35	120	8, 52, 56, 60	
3	Styrene	0.864770	-8.14267	7.57896	418.675	0.288 - 100.51	281.35 <sup>c</sup> -417.92	60.424	21	6	
4	Ethylbenzene	0.859833	-6.85948	5.94339	409.229	0.0204 - 3507.0	243.2 <sup>c</sup> -615.0	78.549	127	8, 17, 56	
5	2-Methyltoluene	0.855257	-6.48662	5.53883	417.496	0.0324 - 3808.0	253.2 <sup>c</sup> -631.64	62.263	127	8, 17, 56	
6	3-Methyltoluene	0.867941	-6.73249	5.87438	412.135	0.0169 - 3650.0	243.2 <sup>c</sup> -619.2	73.326	156	6, 8, 17, 56	
7	4-Methyltoluene	0.847730	-6.39489	5.59094	411.503	0.774 - 3617.0	290.0 <sup>c</sup> -618.2	73.728 <sup>c</sup>	112	8, 17, 56	
8	2-Methylstyrene	0.880379	-7.17666	6.37058	443.504	0.387 - 17.70	305.16 <sup>c</sup> -385.5	28.979	9	4	
9	3-Methylstyrene	0.885861	-7.19653	6.75359	442.985	0.687 - 99.725	314.93 <sup>c</sup> -442.15	28.811	27	4	
10	4-Methylstyrene	0.875061	-7.08160	7.33467	443.748	0.133 - 3078.1	289.15 <sup>c</sup> -443.15	27.919	31	4, 41	
11	n-Propylbenzene	0.891023	-6.89092	5.79948	432.321	0.133 - 3078.1	280.0 <sup>c</sup> -635.0	40.890	91	4, 8	
12	Isopropylbenzene	0.877964	-7.23971	6.06942	425.438	0.057 - 3168.0	264.95 <sup>c</sup> -630.0	49.827	127	6, 8, 16	
13	1-Ethyl-2-ethylbenzene	0.863837	-6.34817	5.19164	438.357	0.141 - 3206.6	285.0 <sup>c</sup> -645.0	34.109	93	4, 8	
14	1-Ethyl-3-ethylbenzene	0.861399	-6.30303	5.19848	434.538	0.118 - 3065.4	280.0 <sup>c</sup> -635.0	38.056	92	4, 8	
15	1-Ethyl-4-ethylbenzene	0.856105	-6.18307	5.09568	435.228	0.120 - 2977.6	280.0 <sup>c</sup> -635.0	37.516	91	4, 8	
16	1,2,3-Trimethylbenzene	0.869047	-6.33423	5.14963	449.175	0.116 - 3283.3	290.0 <sup>c</sup> -660.0	24.677	75	8	
17	1,2,4-Trimethylbenzene	0.846724	-5.41424	4.22211	442.537	0.00886-3076.9	253.0 <sup>c</sup> -645.0	30.109	108	6, 8, 10	
18	1,3,5-Trimethylbenzene	0.872945	-6.55508	5.47586	437.769	0.00938-3046.47	295.0 <sup>c</sup> -645.0	34.219	117	6, 8, 10	
19	n-Butylbenzene	0.889482	-7.01177	6.55027	456.368	0.1120 - 2870.90	295.0 <sup>c</sup> -660.0	19.971	102	4, 8, 41	
20	Isobutylbenzene	0.870338	-6.75481	5.59009	445.940	0.105 - 2775.0	285.0 <sup>c</sup> -645.0	27.785	93	4, 8	
21	sec-Butylbenzene	0.870844	-6.72060	5.52698	446.499	0.101 - 2733.7	285.0 <sup>c</sup> -645.0	27.275	93	4, 8	
22	tert-Butylbenzene	0.881530	-7.21174	6.01764	442.319	0.119 - 2591.4	285.0 <sup>c</sup> -650.0	30.782	90	4, 8	
23	1-Ethyl-2-propylbenzene	0.887506	-6.92315	5.60140	458.002	0.106 - 2827.0	295.0 <sup>c</sup> -660.0	19.014	74	8	
24	1-Ethyl-3-propylbenzene	0.874757	-6.86228	5.30555	455.038	0.128 - 2670.8	295.0 <sup>c</sup> -650.0	25.427	99	2, 8	
25	1-Ethyl-4-propylbenzene	0.882883	-6.86216	5.57573	456.497	0.118 - 2705.5	295.0 <sup>c</sup> -650.0	20.032	100	2, 8	
26	1-Methyl-2-isopropylbenzene	0.877779	-6.88555	5.61774	451.343	0.131 - 2835.9	290.0 <sup>c</sup> -650.0	23.648	109	2, 4, 8	
27	1-Methyl-3-isopropylbenzene	0.875856	-6.90589	5.71011	448.380	0.131 - 2652.8	290.0 <sup>c</sup> -645.0	25.822	107	2, 4, 8	
28	1-Methyl-4-isopropylbenzene	0.875129	-6.86627	5.61507	450.311	0.121 - 2694.2	290.0 <sup>c</sup> -650.0	24.504	107	2, 4, 8	
29	1,2-Diethylbenzene	0.885449	-6.81892	5.48568	456.641	0.112 - 2901.5	295.0 <sup>c</sup> -660.0	19.736	94	4, 8	
30	1,3-Diethylbenzene	0.889714	-6.94128	5.62739	454.362	0.119 - 2716.8	294.85 <sup>c</sup> -650.0	20.954	102	4, 8, 41	
31	1,4-Diethylbenzene	0.893772	-7.13376	5.76066	456.809	0.107 - 2708.6	295.0 <sup>c</sup> -650.0	19.631	93	4, 8	
32	1,2-Dimethyl-3-ethylbenzene	0.868962	-5.88268	4.94042	467.211	0.139 - 2956.5	305.0 <sup>c</sup> -675.0	14.215	102	2, 8	
33	1,2-Dimethyl-4-ethylbenzene	0.888166	-6.72722	5.37774	462.948	0.114 - 2858.4	300.0 <sup>c</sup> -665.0	15.130	101	2, 8	
34	1,3-Dimethyl-2-ethylbenzene	0.891249	-6.82799	5.40578	463.219	0.112 - 2964.6	330.0 <sup>c</sup> -670.0	15.037	101	2, 8	
35	1,3-Dimethyl-4-ethylbenzene	0.892544	-7.08768	4.78949	461.691	0.130 - 2852.5	300.0 <sup>c</sup> -665.0	15.938	101	2, 8	
36	1,4-Dimethyl-5-ethylbenzene	0.867112	-6.04098	4.82215	456.921	0.17 - 2633.7	295.0 <sup>c</sup> -650.0	17.450	99	2, 8	
37	1,2,3,4-Tetramethylbenzene	0.889484	-6.47588	4.96841	460.129	0.101 - 3381.6	295.0 <sup>c</sup> -680.0	17.850	105	2, 8	
38	1,2,3,5-Tetramethylbenzene	0.891876	-6.64575	5.23861	471.208	0.111 - 2970.1	310.0 <sup>c</sup> -690.0	10.058	104	2, 8	
39	1,2,4,5-Tetramethylbenzene	0.884259	-6.36677	4.97446	470.032	0.106 - 2850.3	305.0 <sup>c</sup> -675.0	12.407	102	2, 8	
40	sec-Amylbenzene	0.897853	-6.86006	7.27031	451.128	1.333 - 2913.0	346.75 <sup>c</sup> -675.0	12.868	92	2, 8	
41	3-Ethyl-1-isopropylbenzene	0.859693	-6.82452	7.58198	465.962	0.133 - 101.33	300.95 <sup>c</sup> -451.15	13.585	10	41	
42	3-Ethyl-1-isopropylbenzene	0.871494	-7.16782	8.01142	468.985	0.133 - 101.33	301.45 <sup>c</sup> -446.15	11.582	10	41	
43	3,5-Dimethyltoluene	0.865431	-7.13287	7.83657	472.018	0.133 - 101.33	304.65 <sup>c</sup> -468.95	11.037	10	41	
44	1,2,4-Trimethyl-5-ethylbenzene	0.912511	-5.94151	18.3976	464.965	1.467 - 9.466	360.45 <sup>c</sup> -405.25	12.355	11	41	
45	1,3,5-Trimethyl-2-ethylbenzene	0.782663	-6.86816	4.53769	483.486	1.573 - 101.33	361.65 <sup>c</sup> -483.35	7.6514	11	4	
46	1,2,3,4-Tetramethylbenzene	0.869528	-6.85396	7.42464	482.090	0.133 - 101.33	313.15 <sup>c</sup> -482.15	8.3653	19	4	
47	1,3-Diisopropylbenzene	0.867688	-7.14442	8.11668	475.120	0.133 - 101.33	307.85 <sup>c</sup> -475.15	6.9599	10	41	
48	1,4-Diisopropylbenzene	0.900726	-6.87306	5.22622	483.33	6.753 - 104.63	393.41 <sup>c</sup> -484.73	10.930	10	41	
49	1,2,4-Trimethylbenzene	0.881965	-7.59082	8.58854	491.389	0.133 - 101.33	319.15 <sup>c</sup> -491.15	8.6840	7	4	
50	1,3,4-Trimethylbenzene	0.879248	-6.92921	7.78309	490.542	0.133 - 101.33	321.05 <sup>c</sup> -490.65	6.5820	10	41	
51	Hexamethylbenzene	1.00973	-5.04725	-6.30130	571.163	0.00028 <sup>c</sup> -0.0144	303.10 <sup>c</sup> -343.02	6.3034	10	41	
52								0.6701	9	48	

<sup>a</sup> P in atm (1.01325 bar or 101.32 kPa); K in T.

<sup>b</sup> AAD = absolute average deviation =  $\frac{\sum |\text{Calculated value} - \text{experimental value}|}{\text{number of data points}}$

<sup>c</sup> 400 K outside the temperature range of the data used in evaluating the coefficient of the vapor pressure equation.

TABLE 11. Coefficients of vapor pressure equation and the calculated vapor pressure at 400 K for naphthalene and its derivatives

No.	Name	$\log_{10} P = (A - D/T) \times 10 (A + BT + CT^2)^a$				Vapor Pressure Range, kPa	Temperature Range, K	Calculated Vapor Pressure kPa at 400.0 K	AAD <sup>b</sup> %	Number of Data Points	Data Reference Number
		A	B x 10 <sup>4</sup>	C x 10 <sup>7</sup>	D						
1	Naphthalene	0.832267	-4.41855	2.89627	490.988	0.5253 - 4045.4	340.15-751.65	7.2571	0.815	86	4, 6
2	1-Methylnaphthalene	0.863323	-5.26355	3.75850	517.727	0.00176-7415.36	278.85-593.38	3.0627	0.366	93	2, 6, 53
3	2-Methylnaphthalene	0.879050	-5.85793	4.19253	514.242	1.33300-7354.96	378.00-529.32	3.4264	0.195	89	2, 4, 6, 53
4	2-Ethyl-naphthalene	0.923623	-6.97505	5.07450	531.480	1.33300-199.98	393.15-565.45	1.8090	0.0358	27	2
5	1-Ethyl-naphthalene	0.871612	-5.23140	3.70623	531.189	0.00153-199.98	286.20-565.05	1.8964	0.932	34	2, 28
6	1,2-Dimethylnaphthalene	0.950015	-6.99660	4.52556	539.430	1.33300-106.66	402.35-541.75	1.1990 <sup>c</sup>	0.113	23	2
7	1,3-Dimethylnaphthalene	1.72680	-7.87991	-4.2.8535	540.353	1.33300-103.99	400.00-541.00	1.3768	1.68	13	2
8	1,4-Dimethylnaphthalene	1.97594	-8.55425	-59.4189	544.362	1.33300-103.99	397.00-544.00	1.8453	2.27	13	2
9	1,8-Dimethylnaphthalene	0.951477	-8.49048	2.61743	576.908	0.0148 - 1.8032	328.15-713.15	1.0306	1.89	20	38
10	2,3-Dimethylnaphthalene	1.09999	-10.2378	-11.3931	631.969	0.01400-1.8534	333.15-710.15	1.3707	3.92	16	38
11	2,6-Dimethylnaphthalene	1.14901	-11.9220	-17.3468	687.081	0.0536-3.4439	328.15-718.15	1.6799	5.60	15	38
12	2,7-Dimethylnaphthalene	1.11518	-10.6526	-13.2234	632.459	0.01987-1.5037	333.15-398.15	1.8228 <sup>c</sup>	5.87	15	38
13	1-r-Propylnaphthalene	1.01439	-7.21205	0.034076	546.126	1.33300-101.33	403.15-545.95	1.1476 <sup>c</sup>	0.525	10	2
14	2-r-Propylnaphthalene	1.02538	-7.12594	-0.699309	546.808	1.33300-101.33	404.15-546.65	1.0928 <sup>c</sup>	0.557	10	2
15	1-Isopropylnaphthalene	0.946045	-6.97957	4.44862	540.864	1.33300-199.98	402.45-575.15	1.2000 <sup>c</sup>	0.255	27	2
16	2-Isopropylnaphthalene	0.951658	-7.02612	3.90232	541.304	1.33300-199.98	401.65-577.15	1.2452 <sup>c</sup>	0.307	27	2
17	1,3,5-Trimethylnaphthalene	1.01709	-6.95334	0.567876	557.950	1.33300-101.33	415.15-557.65	0.62396 <sup>c</sup>	0.846	8	2
18	1,3,7-Trimethylnaphthalene	1.03964	-7.09533	-1.37129	553.629	1.33300-101.33	409.15-553.15	0.84060 <sup>c</sup>	0.389	7	2
19	1,4,5-Trimethylnaphthalene	0.998467	-7.03095	1.71081	558.187	1.33300-101.33	415.15-558.15	0.64463 <sup>c</sup>	1.20	7	2
20	1-r-Butylnaphthalene	1.10895	-7.77663	-4.60035	563.025	1.33300-106.66	412.85-565.95	0.70084 <sup>c</sup>	1.28	23	2
21	2-r-Butylnaphthalene	0.971423	-6.86834	3.12197	561.352	1.33300-106.66	418.15-564.15	0.56340 <sup>c</sup>	0.848	28	2
22	1-tert-Butylnaphthalene	0.916603	-4.48364	-0.616268	551.533	1.33300-106.66	407.15-554.15	0.96225 <sup>c</sup>	0.643	23	2
23	2-tert-Butylnaphthalene	0.930573	-5.27602	0.144968	553.378	1.33300-106.66	407.15-556.15	0.96730 <sup>c</sup>	0.665	23	2

<sup>a</sup> P in atm (1.01325 bar or 101.325 kPa); T in K.

<sup>b</sup> AAD = absolute average deviation =  $\sum \frac{|\text{Calculated value} - \text{experimental value}|}{\text{experimental value}}$  / number of data points

<sup>c</sup> 400 K outside the temperature range of the data used in evaluating the coefficients of the vapor pressure equation.

Table 12. Coefficients of vapor pressure equation and the calculated vapor pressure at 40°C K for saturated ring-compounds

No.	Name	$\log_{10} P = (1 - D/T) \times 10^{(A+BC/T^2)}$ <sup>a</sup>			Vapor Pressure Range, kPa	Temperature Range, K	AAD <sup>b</sup> %	Number of Data Points	Reference Number	Pressure kPa at 40°C K
		A	B x 10 <sup>4</sup>	C x 10 <sup>7</sup>						
1	Cyclopropane	0.764677	-6.98761	9.83198	1.333-5579.5	171.85-398.3	0.188	65	2, 4, 54	5734.5 <sup>c</sup>
2	Cyclobutane	0.887736	-15.11134	24.6051	0.133-199.98	181.15-305.66	0.770	62	2, 4, 41, 70	2307.9 <sup>c</sup>
3	Methylcyclobutane	0.861895	-10.8963	10.8762	0.133-101.33	177.15-277.65	0.021	10	41	1657.7 <sup>c</sup>
4	Cyclopentane	0.818603	-7.52365	8.27395	0.043-4039.0	193.20-503.20	0.574	85	4, 15, 17, 50	745.63
5	Cyclohexane	0.881199	-9.58655	9.72305	0.133-4074.8	227.85-553.64	0.877	140	2, 4, 6, 17, 41, 46, 47, 50	336.61
6	Methylcyclopentane	0.872156	-8.88031	10.8367	0.0019-2924.0	183.15-513.15	0.848	60	2, 4, 17	119.03
7	Cycloheptane	0.865524	-8.19621	7.88065	1.333-270.11	284.35-432.17	0.396	42	2, 4, 17	125.64
8	Ethylcyclopentane	0.839111	-7.11414	6.79853	1.333-3143.0	273.24-568.15	0.151	77	2, 4, 17	188.49
9	1,1-Dimethylcyclopentane	0.833976	-10.8001	12.4624	0.026-561.37	213.15-433.15	1.522	70	2, 4, 17	272.69
10	1,cis-2-Dimethylcyclopentane	0.888150	-8.36884	6.19165	4.00-199.98	201.15-398.35	1.631	45	2, 4, 17	205.66 <sup>c</sup>
11	1,trans-2-Dimethylcyclopentane	0.849952	-8.27119	8.67505	1.333-199.98	264.15-390.25	0.044	45	2, 4, 17	253.26 <sup>c</sup>
12	1,cis-3-Dimethylcyclopentane	0.835365	-8.20938	10.1173	1.333-199.98	263.15-389.15	1.40	46	2, 4, 17	263.71 <sup>c</sup>
13	1,trans-3-Dimethylcyclopentane	0.833033	-8.40781	7.45113	1.333-199.98	263.15-390.15	1.399	46	2, 4, 17	249.84 <sup>c</sup>
14	Methylcyclohexane	0.862568	-8.71426	8.69688	0.0036-3116.0	203.20-563.20	0.682	115	2, 4, 6, 17	198.91
15	Ethylcyclohexane	0.877363	-8.63498	8.47613	0.033-310.80	243.20-453.20	0.394	57	2, 4, 17, 41	88.698
16	1,1-Dimethylcyclohexane	0.803626	-5.30532	3.8510	0.133-199.98	248.75-430.25	0.346	57	2, 4, 41	122.71
17	1,cis-2-Dimethylcyclohexane	0.81813	-5.6619	5.0185	0.133-199.98	257.05-430.72	0.470	57	2, 4, 41	93.002
18	1,trans-2-Dimethylcyclohexane	0.827486	-5.32608	4.53266	0.133-199.98	252.05-430.72	1.170	37	2, 4, 41	121.04
19	1,cis-3-Dimethylcyclohexane	0.81956	-7.14598	3.99346	0.133-199.98	260.05-430.52	0.137	37	2, 4, 41	121.04
20	1,trans-3-Dimethylcyclohexane	0.840923	-6.83912	5.07104	0.133-199.98	253.75-430.52	0.139	37	2, 4, 41	107.59
21	1,cis-4-Dimethylcyclohexane	0.826453	-6.73308	2.74765	0.133-199.98	268.05-424.95	0.230	37	2, 4, 41	108.44
22	1,trans-4-Dimethylcyclohexane	0.856653	-6.73308	8.50105	0.133-199.98	268.05-424.95	0.187	37	2, 4, 41	123.39
23	Isopropylcyclopentane	0.861793	-8.16102	8.29788	1.333-199.98	269.25-426.95	0.032	47	2, 4, 41	102.48
24	Propylcyclopentane	0.856193	-8.16102	8.29788	1.333-199.98	294.75-431.35	0.051	46	2, 4, 41	90.639
25	1-Ethyl-1-methylcyclopentane	0.852522	-7.84448	6.25954	0.028-270.02	238.15-288.15	0.391	52	2, 4, 34	116.55
26	cis-2-Ethyl-1-methylcyclopentane	0.852851	-7.84448	5.94712	0.028-1114	279.53-431.35	0.234	11	34	119.41 <sup>c</sup>
27	1,1,2-Trimethylcyclopentane	0.853137	-8.19842	8.40843	1.333-199.98	272.85-404.45	0.026	46	2, 4, 41	143.08
28	1,1,3-Trimethylcyclopentane	0.848231	-8.28174	8.81168	1.333-199.98	313.35-458.95	0.184	46	2, 4, 41	179.97
29	Propylcyclohexane	0.865420	-7.40426	5.98962	6.41-104.01	343.66-428.75	0.013	20	2, 4, 41	44.499
30	Isopropylcyclohexane	0.876667	-7.99142	7.47343	9.59-269.98	348.31-464.42	0.011	20	2, 4, 41	47.502
31	cis-3-Ethyl-1-methylcyclohexane	0.843964	-6.42051	5.49912	6.40-104.00	327.82-40.80	0.286	25	34	56.223
32	1,1,3-Trimethylcyclohexane	0.838270	-6.63916	5.61172	1.333-199.98	332.65-484.35	0.061	21	2, 4, 41	78.174
33	n-Butylcyclohexane	0.891776	-7.48841	6.21822	6.41-104.01	376.61-453.57	0.021	27	2, 4, 41	47.514
34	Isobutylcyclohexane	0.848267	-6.44098	5.35931	6.41-104.01	376.61-453.57	1.37	20	2, 4, 41	23.314
35	sec-Butylcyclohexane	0.925582	-7.33653	2.83949	6.41-104.00	357.18-445.82	0.022	20	2, 4, 41	29.609
36	tert-Butylcyclohexane	0.862098	-7.99999	7.51667	6.40-104.00	357.18-445.82	0.022	20	2, 4, 41	29.609

<sup>a</sup> P in Atm(1.01325 bar or 101.325 kPa); T in K

<sup>b</sup> AAD = absolute average deviation =  $\frac{\sum | \text{Calculated value} - \text{experimental value} |}{\text{number of data points}}$

<sup>c</sup> 4000 K is outside the temperature range of the data used in evaluating the coefficients of the vapor pressure equation.



Table 13. Coefficients of vapor pressure equation and the calculated vapor pressure at 400 K for unsaturated ring compounds

No.	Name	$\log_{10} P = (A - D/T) \times 10^{(A+B+CT)^a}$				Vapor Pressure Range, kPa	Temperature Range, K	AAD <sup>b</sup> %	Number of Data Points	Reference Number	Pressure kPa, at 400 K
		A	B x 10 <sup>4</sup>	C x 10 <sup>7</sup>	D						
1	Cyclobutene	0.822553	-10.9389	18.2344	275.824	0.667-101.33	189.75-275.55	1.05	21	4, 41	3024.4 <sup>c</sup>
2	1,3-Cyclopentadiene	0.919018	-8.68344	-3.41259	314.762	18.82-46.33	271.25-313.05	0.055	20	15	508.86 <sup>c</sup>
3	Cyclopentene	0.814441	-7.42372	8.49035	317.520	0.852-743.8	223.2-393.2	0.459	22	17, 71	858.79 <sup>c</sup>
4	1,3-Cyclohexadiene	0.823433	-6.73214	6.67096	353.486	16.80-135.20	303.96-363.31	0.152	19	27, 31	345.40 <sup>c</sup>
5	1,4-Cyclohexadiene	0.916704	-6.81678	-7.02362	368.566	11.89-45.25	304.25-322.23	0.206	17	27	187.51 <sup>c</sup>
6	Cyclohexene	0.873674	-9.73841	10.9078	356.172	0.0328-129.63	213.20-364.53	0.265	39	17, 27, 31	319.90 <sup>c</sup>
7	Indane	0.796974	-5.93769	9.52748	455.041	0.133-104.41	289.55-456.97	1.46	20	6, 41	19.990
8	Indene	0.859420	-6.08324	4.77502	451.051	4.34-104.41	335.01-452.24	0.169	50	6, 26, 37	23.825
9	Tetralin	0.859186	-5.72417	4.41971	480.364	0.133-3564.64	311.15-710.93	1.589	46	4, 16, 32, 41, 73	9.9861
10	cis-Decalin	0.683577	-9.90094	-2.28555	468.915	0.133-1571.48	295.65-727.59	2.136	46	4, 16, 32, 41, 73	14.969
11	trans-Decalin	0.860979	-6.38749	4.59180	460.458	0.253-102.73	365.51-461.02	0.463	19	37	19.233
12	1,1-Dimethylindan	0.869995	-6.14831	4.52781	467.243	5.53-47.38	313.15-467.22	0.037	24	37	14.780
13	4,6-Dimethylindan	0.887063	-6.04521	4.35551	498.089	0.050-47.38	313.15-469.96	0.144	18	37	5.4159
14	4,7-Dimethylindan	0.887652	-6.04765	4.32553	501.078	0.050-47.38	313.15-469.96	0.160	17	37	4.9525
15	Biphenyl	1.11763	-8.13240	-13.7006	601.351	0.027-1.835	342.35-673.15	4.28	15	56	1.3564
16	Phenylcyclohexane	0.821410	-8.73337	1.02285	528.437	0.104-1103.57	342.35-673.15	1.298	87	6, 72	1.3288
17	Bicyclohexyl	0.914718	-8.43553	6.82927	508.790	264.8-2457.3	500.30-727.59	0.617	29	73	4.822 <sup>c</sup>
18	1,1-Dicyclohexylethane	0.876522	-8.41554	3.04965	510.920	0.065-349.09	321.20-571.25	0.859	28	1, 44	3.9703
19	1-Phenylcyclohexylethane	1.31737	-14.8631	14.2837	521.584	0.067-353	343.15-727.59	7.888	5	1, 16, 44, 73	0.19413
20	Bi-phenylmethane	0.918947	-6.38483	4.28913	557.844	0.067-353	343.15-727.59	1.635	5	1	3.3609
21	1,1,4,6-Tetramethylindan	0.908238	-6.33083	4.2020	568.943	0.065-821.0	313.15-468.80	0.482	18	37	3.0528
22	1,1,4,7-Tetramethylindan	0.895344	-6.33098	4.01520	597.025	0.032-36.565	313.15-468.80	0.186	18	37	0.96348
23	Bi-phenylethane	1.03345	-9.0266	20.9310	574.786	0.025-31.177	359.05-404.05	0.384	5	1	1.0761
24	1-Phenylphenylethane	0.89340	-5.42680	8.02993	524.404	0.067-333	359.05-404.05	0.524	5	1	0.80338
25	2-Phenylphenylethane	0.917694	-6.08631	5.17356	524.981	0.067-333	359.05-404.05	0.403	5	1	0.80338
26	Ethylphenylethane	0.80357	-5.08471	3.29969	524.979	0.067-333	359.05-404.05	0.219	5	1	1.0079
27	1-Cyclohexyl-1-phenylethane	1.08957	-15.3344	24.1341	507.179	0.067-333	348.15-406.15	0.667	5	1	1.0064
28	2-Cyclohexyl-1-phenylethane	1.08923	-16.0392	22.9852	528.286	0.067-333	348.15-406.15	0.701	5	1	1.1995
29	1-Cyclohexyl-1-phenylpropane	1.07456	-16.0336	22.6955	528.173	0.067-333	348.15-406.15	0.594	5	1	1.1848
30	1,1-Dicyclohexylethane	1.07652	-15.8050	23.4332	516.862	0.067-333	348.15-406.15	0.972	5	1	
31	1,2-Dicyclohexylethane	1.07728	-15.4160	24.9170	506.850	0.067-333	348.15-406.15		5	1	

<sup>a</sup> P in atm(1.01325 bar or 101.325 kPa); T in K  
<sup>b</sup> AAD = absolute average deviation =  $\frac{\sum | \text{Calculated value} - \text{experimental value} |}{\text{number of data points}}$  / experimental value  
<sup>c</sup> 400K is outside the temperature range of the data used in evaluating the coefficients of the vapor pressure equation.

Table 14. Coefficients of vapor pressure equation and the calculated vapor pressure at 400 K for sulfur compounds

no.	Name	$\log_{10} P = (1 - D/T) \times 10^4 (A + B \times 10^{-4} + C \times 10^{-7} + D)$				Vapor Pressure Range, kPa	Temperature Range, K	AAD <sup>b</sup> %	Number of Data Points	Reference Number	Pressure kPa at 400 K
		A	B x 10 <sup>-4</sup>	C x 10 <sup>-7</sup>	D						
1	Thiacyclopropane	0.823181	-7.01267	7.70188	328.076	1.333-270.11	238.55-360.88	0.051	40	2, 4	630.01 <sup>c</sup>
2	Thiacyclobutane	0.860604	-9.57208	10.35166	368.152	1.333-270.11	268.23-404.79	0.090	57	2, 4, 36	240.84
3	Thiophene	0.901276	-10.3229	11.5393	394.395	1.333-270.11	287.33-431.60	0.436	61	2, 36, 43	118.22
4	Tetrahydrothiophene	0.831037	-7.11948	6.89859	394.281	1.333-199.98	287.33-420.61	0.134	32	2, 24	118.47
5	Thiacyclopentane	0.865149	-7.93338	7.59224	357.255	0.107-5467.15	228.13-577.61	1.354	145	2, 4, 6, 16, 41, 51	319.69
6	2-Methylthiophene	0.943733	-10.3914	11.2735	385.680	1.333-199.98	282.13-411.15	0.250	35	2, 24	150.13
7	3-Methylthiophene	0.803952	-5.13436	5.45365	388.532	1.333-199.98	248.65-411.15	1.385	45	2, 24, 41	139.58
8	Cyclopentanethiol	0.928892	-10.4911	10.6839	405.333	19.920-270.11	354.02-445.93	0.061	30	4, 36	87.572
9	2-Methylthiacyclopentane	0.898551	-9.69558	10.5617	405.832	1.333-270.11	295.87-446.24	0.716	65	2, 36, 43	86.294
10	3-Methylthiacyclopentane	0.913016	-10.2124	10.9071	411.706	1.333-270.11	300.25-452.63	0.457	65	2, 36, 43	73.444
11	Thiacyclohexane	0.914589	-10.2766	10.8708	414.929	1.333-199.98	302.35-443.15	0.106	48	2, 4, 43	67.317
12	Benzethiol	0.928694	-9.23421	8.59363	442.321	1.333-270.11	235.43-485.11	0.075	57	2, 4, 36	20.152
13	2,5-Dimethylthiophene	0.885251	-10.3540	14.59835	407.929	7.40-34.26	333.45-371.45	0.047	5	24	80.141 <sup>c</sup>
14	2-Ethylthiophene	0.868809	-10.2829	16.6827	404.508	8.12-37.33	333.45-371.45	0.038	5	24	88.307 <sup>c</sup>
15	Cyclohexanethiol	0.922485	-10.1571	10.0208	431.996	9.582-270.11	356.89-475.80	0.082	21	36	42.258
16	2, cis-5-Dimethylthiacyclopentane	0.916043	-10.2115	10.6693	415.741	1.333-199.98	303.15-444.15	0.222	45	2, 43	65.782
17	2, trans-5-Dimethylthiacyclopentane	0.911961	-10.3802	11.2368	415.203	1.333-199.98	302.15-443.15	0.268	40	2, 43	66.782
18	2-Methylthiacyclohexane	0.892566	-9.26534	9.58365	426.209	1.333-199.98	309.15-455.15	0.221	50	2, 43	49.601
19	3-Methylthiacyclohexane	0.903042	-9.76615	10.3670	431.193	1.333-199.98	313.15-460.15	0.176	44	2, 43	43.048
20	4-Methylthiacyclohexane	0.918744	-10.2913	10.5693	431.815	1.333-199.98	314.15-461.15	0.181	48	2, 43	42.496
21	2-Methylbenzenethiol	0.921152	-8.62878	7.84882	467.376	1.333-199.98	343.15-498.15	0.361	27	2	13.851
22	3-Methylbenzenethiol	0.958438	-10.1375	9.47433	468.259	1.333-199.98	343.15-498.15	0.203	27	2	14.402
23	4-Methylbenzenethiol	0.922351	-8.74250	7.84906	468.114	1.333-199.98	343.15-498.15	0.315	27	2	14.313
24	1-Thiethylbenzene	0.884670	-6.07526	4.25882	467.456	9.582-70.11	390.25-452.97	0.011	13	4, 9	13.716
25	1-Naphthalenethiol	1.14267	-16.7242	17.1057	559.324	0.20-101.33	379.15-559.15	1.424	6	9	0.62485 <sup>c</sup>
26	2-Naphthalenethiol	0.865090	-6.20254	7.97377	559.174	1.373-101.33	419.45-559.15	1.820	6	9	0.62485 <sup>c</sup>
27	Dibenzothiophene	0.865373	-5.51221	6.05701	605.160	0.471-105.90	424.81-607.53	0.405	19	75	0.14877 <sup>c</sup>

<sup>a</sup> P in Atm (1.01325 bar or 101.325 kPa); T in K

<sup>b</sup> AAD = Absolute average deviation =  $\frac{\sum |\text{Calculated value} - \text{experimental value}|}{\text{number of data points}}$

<sup>c</sup> 400 K is outside the temperature range of the data used in evaluating the coefficients of the vapor pressure equation.

TABLE 13. Coefficients of vapor pressure equation and the calculated vapor pressures at 400 K for nitrogen compounds - I

No.	Name	A	B x 10 <sup>4</sup>	C x 10 <sup>7</sup>	D	Vapor Pressure Range, kPa	Temperature Range, K	Vapor Pressure kPa	AD <sup>b</sup>	Number of Data	Data Reference Numbers
1	Aziridine	0.805550	-3.53813	3.93398	328.480	0.017-9363.2	175.0-520.0	910.44	0.5580	70	8
2	Azoxidine	0.846557	-3.47000	4.85057	333.317	0.001-9359.7	200.0-945.0	0.2138	0.7238	143	8, 24, 39, 35, 51
3	Cyrtolidine	0.860256	-6.05913	5.07226	329.916	0.011-8932.3	215.0-925.0	0.1313	0.4258	143	4, 8, 35, 51
4	Pyridine	0.846892	-6.09912	5.15399	388.392	0.039-549.6	140.0-300.0	0.7488	0.181	127	4, 8, 16, 35, 51
5	2-methylpyrrole	0.880560	-7.23818	6.42262	385.382	0.016-4799.5	230.0-595.0	1.4030	0.7488	103	8, 24, 35
6	Piperidine	0.885414	-7.91475	6.97866	379.377	0.015-4388.7	265.0-590.0	1.7836	0.6942	100	8, 16, 35
7	Aniline	0.911551	-6.64936	5.15455	267.025	0.008-5165.0	267.0-590.0	0.9436	0.6942	130	4, 6, 8, 16
8	2-methylpyridine	0.887914	-7.70705	6.85261	402.320	0.001-4545.9	215.0-620.0	94.920	1.4087	156	4, 6, 8, 16, 35
9	3-methylpyridine	0.865977	-6.48542	5.41256	417.217	0.035-4650.0	250.0-645.0	0.1687	0.1687	141	4, 8, 16, 35
10	4-methylpyridine	0.862538	-6.32828	5.24419	418.461	0.234-4548.2	280.0-645.0	59.971	0.1155	115	4, 8, 16, 35
11	2,5-dimethylpyrrole	0.875279	-8.18064	6.24150	440.662	0.002-5037.7	255.0-660.0	0.4274	0.4274	102	16
12	Cyclohexylamine	0.848474	-5.99285	5.24860	406.825	7.843-86.06	333.9-401.5	83.487	0.4113	15	8, 35
13	2-methylpiperidine	0.890367	-8.35931	7.50471	391.355	0.441-3666.3	270.0-595.0	128.30	0.1978	86	8, 35
14	2-methylpyrrolidine	0.910765	-6.64743	5.27032	457.650	0.017-4745.4	250.0-685.0	121.306	0.1978	86	8, 35
15	3-methylpyrrolidine	0.869393	-6.12111	4.92265	418.461	0.007-3628.4	240.0-670.0	121.306	0.1978	86	8, 35
16	4-methylpyrrolidine	0.843038	-5.13221	4.02456	438.546	0.007-3628.4	240.0-670.0	121.306	0.1978	86	8, 35
17	2-methylpyridine	0.887914	-7.70705	6.85261	402.320	0.001-4545.9	215.0-620.0	94.920	1.4087	156	4, 6, 8, 16, 35
18	3-methylpyridine	0.865977	-6.48542	5.41256	417.217	0.035-4650.0	250.0-645.0	0.1687	0.1687	141	4, 8, 16, 35
19	4-methylpyridine	0.862538	-6.32828	5.24419	418.461	0.234-4548.2	280.0-645.0	59.971	0.1155	115	4, 8, 16, 35
20	2,4-dimethylpyridine	0.887114	-6.47984	5.39796	430.124	0.026-3721.5	270.0-620.0	0.1021	0.1021	104	8, 16
21	2,5-dimethylpyridine	0.885281	-7.15067	6.18999	417.136	0.106-3721.5	270.0-680.0	0.1448	0.1448	94	8, 16
22	2,6-dimethylpyridine	0.873502	-6.18582	4.84358	452.235	0.019-3951.1	270.0-680.0	0.1543	0.1543	95	4, 8
23	3,4-dimethylpyridine	0.871062	-6.21188	4.99649	445.022	0.018-3847.1	265.0-665.0	0.1231	0.1231	92	4, 8
24	N-methylamine	0.921600	-6.99135	5.63532	468.447	0.011-4693.7	280.0-710.0	0.5250	0.5250	90	8, 41
25	2-methylamine	0.907135	-6.44774	4.94693	473.369	0.049-4649.9	300.0-710.0	0.2815	0.2815	90	8, 41
26	3-methylamine	0.923479	-6.91988	5.41104	476.329	0.007-4399.1	280.0-705.0	0.3243	0.3243	93	4, 8
27	4-methylamine	0.938651	-6.57024	5.71261	455.445	0.022-4443.4	285.0-720.0	0.3445	0.3445	88	8
28	1-methylpyrrolidine	0.887914	-7.70705	6.85261	402.320	0.001-4545.9	215.0-620.0	94.920	1.4087	156	4, 6, 8, 16, 35
29	2-methylpyrrolidine	0.865977	-6.48542	5.41256	417.217	0.035-4650.0	250.0-645.0	0.1687	0.1687	141	4, 8, 16, 35
30	3-methylpyrrolidine	0.862538	-6.32828	5.24419	418.461	0.234-4548.2	280.0-645.0	59.971	0.1155	115	4, 8, 16, 35
31	4-methylpyrrolidine	0.843038	-5.13221	4.02456	438.546	0.007-3628.4	240.0-670.0	121.306	0.1978	86	8, 35
32	N,N-dimethylamine	0.909397	-7.07673	5.69581	466.445	0.014-3721.2	275.0-710.0	0.4667	0.4667	83	8
33	2,4-dimethylamine	0.926009	-6.89676	5.31053	490.122	0.004-3202.6	250.0-660.0	0.6847	0.6847	88	8
34	2,6-dimethylamine	0.845606	-5.35481	4.28671	451.482	0.004-3272.6	285.0-720.0	0.223	0.223	80	8
35	2-methyl-5-ethylpyridine	0.846954	-5.46549	4.48622	443.588	0.006-3200.0	250.0-640.0	0.323	0.323	77	8
36	2,4,6-trimethylpyridine	0.840733	-5.47228	4.49971	436.593	0.023-3232.8	260.0-640.0	35.783	0.453	141	4, 8
37	2-methyl-5-ethylpiperidine	0.901210	-6.33889	4.26359	516.182	0.009-4479.0	300.0-800.0	3.1428	0.520	127	4, 8
38	Isoquinoline	0.897177	-6.73559	4.69070	510.552	0.006-3731.5	290.0-780.0	4.0885	0.520	127	4, 8
39	Quinoline	0.884718	-6.66541	5.73271	500.141	0.113-101.3	333.2-500.2	3.9669	0.730	10	41
40	4-Cumidine	0.901277	-6.32720	4.83752	498.038	0.003-3238.6	280.0-715.0	5.0441	0.329	88	8
41	4-Isopropylamine	0.890841	-6.76937	5.40004	458.592	0.003-3223.7	339.4-665.0	18.060	0.481	90	8, 41
42	N,N,2-trimethylamine	0.924688	-6.88109	4.82176	482.716	0.003-3750.0	275.0-695.0	7.5222	0.424	95	8
43	N,N,4-trimethylamine	0.909200	-6.02186	4.52608	507.562	0.154-3500.0	340.0-670.0	3.3522	0.376	78	8
44	2,4,5-trimethylamine	0.959525	-7.30332	4.89518	526.133	0.010-4956.9	330.0-905.0	1.7778	0.399	120	4, 8
45	3-methylisocytosine	0.936276	-6.69538	4.65103	520.768	0.004-4800.8	300.0-785.0	2.1653	0.352	98	8
46	2-methylquinoline	0.951188	-6.50942	4.37314	538.672	0.007-4554.4	325.0-795.0	0.318	0.318	98	8
47	3-methylquinoline	0.971408	-7.84250	5.29478	538.063	0.009-3628.2	320.0-795.0	1.2541	0.413	122	4, 8
48	6-methylquinoline	0.942392	-6.45934	4.37190	530.777	0.023-4654.7	330.0-790.0	1.4135	0.278	110	4, 8
49	7-methylquinoline	0.928604	-6.32078	4.26965	520.971	0.006-4950.8	305.0-790.0	0.328	0.328	115	4, 8
50	8-methylquinoline	0.822931	-2.94554	2.19845	574.066	0.005-385.56	325.0-645.0	0.40996	0.324	65	8
51	1-methylamine	0.860256	-4.44286	3.71453	579.422	0.161-351.60	385.0-645.0	0.33845	0.307	53	8
52	2-methylamine	0.890722	-6.35906	6.06802	520.647	0.001-101.62	281.9-521.0	2.3606	0.567	50	8
53	Quinaldine	0.923880	-7.08036	5.70974	489.409	0.004-1684.20	305.0-645.0	6.9057	0.286	74	4, 8
54	N-Dimethylamine	0.981169	-8.10352	5.44560	540.159	0.002-3826.2	305.0-805.0	1.1524	0.705	120	4, 8
55	2,4-Dimethylquinoline	0.962391	-7.46854	4.94350	538.435	0.004-3753.3	310.0-800.0	0.443	0.443	126	4, 8
56	2,6-Dimethylquinoline	0.879484	-5.71717	4.32562	575.017	0.005-556.62	338.0-785.0	0.583	0.583	85	8, 34
57	3-methylamine	0.938990	-6.17158	4.32562	575.017	0.005-556.62	338.0-785.0	0.583	0.583	85	8, 34
58	Piperazine	0.839896	-4.19344	3.63487	618.827	0.133-101.33	402.6-519.2	0.920	0.920	10	41
59	Acridine	0.913570	-5.42806	5.55168	555.168	0.133-101.33	376.7-555.2	0.46343	0.695	10	41
60	Methyldiphenylamine	0.906637	-4.74302	3.73341	595.800	0.002-7.015	347.8-373.8	2.04	2.04	7	42
61	N-Ethylcarbazol	0.910264	-5.67107	3.81118	569.073	0.003-583.05	320.0-670.0	0.45449	0.391	70	8
62	N-Ethylidiphenylamine	0.924113	-5.87692	4.40076	583.802	0.011-492.57	350.0-670.0	0.23169	0.222	65	8
63	Dibenzylamine	0.920504	-5.87692	3.95486	566.122	0.004-623.62	325.0-670.0	0.47251	0.557	70	8

<sup>a</sup> P in atm (1.01325 bar or 101.325 kPa); T in K.

<sup>b</sup> AD = absolute average deviation =  $\frac{\sum | \text{Calculated value} - \text{experimental value} |}{\text{number of data points}}$

<sup>c</sup> 400 K outside the temperature range of the data used in evaluating the coefficients of the vapor pressure equation.

TABLE 16. Coefficients of vapor pressure equation and the calculated vapor pressures at 400 K for nitrogen compounds - II

No.	Name	$\log_{10} P = (1-D/T) \times 10^4 (A + BT + CT^2)^a$				Vapor Pressure Range, kPa	Temperature Range, K	Vapor Pressure at 400.0 K, kPa	AAD % <sup>b</sup>	Number of Data	Data Reference Numbers
		A	Bx10 <sup>4</sup>	Cx10 <sup>7</sup>	D						
1	Pyrazine	0.844138	-5.83079	4.89556	388.651	12.755-5673.0	330.0-620.0	139.46	0.0637	59	8
2	Piperazine	0.778574	-3.64705	2.83758	419.081	0.165-4553.3	270.0-655.0	60.034	0.550	61	8
3	2-methylpyrazine	0.841770	-5.57164	4.63670	411.160	2.392-4777.6	310.0-630.0	82.399	0.0324	65	8
4	1-methylpiperazine	0.844192	-5.70303	4.79143	438.398	1.168-4550.0	300.0-630.0	73.676	0.0460	67	8
5	1,3-Diaminobenzene	0.938599	-5.86839	4.04968	558.167	0.012-1578.7	340.0-720.0	0.48363	0.148	77	8
6	1,3-Phenylenediamine	0.896276	-5.49204	5.11780	558.585	0.133-101.33	373.0-558.7	0.53987	0.284	10	41
7	Phenyldiazine	0.883884	-5.47784	6.06346	515.158	0.133-101.33	345.0-491.4	2.1990	1.01	9	41
8	cis-2,5-Dimethylpiperazine	0.845668	-5.70303	4.79143	438.398	0.396-3000.0	300.0-635.0	33.961	0.0434	68	8
9	4-amino-2,6-dimethylpyridine	0.915517	-5.83468	4.24064	519.085	20.251-3820.7	460.0-745.0	2.146	0.106	58	8
10	2,4-Diaminotoluene	0.937286	-5.67652	3.87010	565.108	0.091-1440.6	375.0-720.0	0.36568	0.0805	70	8
11	Tetramethylpiperazine	0.845378	-5.69793	4.73789	455.533	0.201-2488.2	300.0-645.0	20.922	0.0488	70	8
12	1-Phenylpiperazine	0.869801	-4.18652	2.62681	559.666	0.002-561.3	310.0-655.0	0.61654	0.404	70	8
14	Azobenzene	0.894170	-5.64849	5.36386	566.301	0.133-101.33	316.7-566.2	0.44244	0.461	10	41
15	DL-(4-aminophenyl)methane	0.955651	-4.42562	2.43881	657.679	0.006-325.17	400.0-720.0	0.59230	0.605	65	8
16	Isoxazole	0.908474	-9.18057	8.98973	368.513	0.003-3741.8	205.0-550.0	243.74	0.588	70	8
17	Oxazole	0.917157	-10.4622	11.2062	342.718	0.005-3629.1	195.0-510.0	487.46	0.260	64	8
18	2-nitrophenol	0.885400	-6.30106	6.42864	487.905	0.133-101.33	322.5-487.7	6.4344	0.581	10	41

<sup>a</sup> p in atm (1.01325 bar or 101.325 kPa); T in K.

<sup>b</sup> AAD = absolute average deviation =  $\frac{1}{n} \left| \frac{\text{Calculated value} - \text{experimental value}}{\text{experimental value}} \right|$  number of data points

<sup>c</sup> 400 K outside the temperature range of the data used in evaluating the coefficients of the vapor pressure equation.

# VAPOR PRESSURE OF COAL CHEMICALS

TABLE 17. Coefficients of Vapor Pressure Equation and the Calculated Vapor Pressure at 400 K for Oxygen Compounds - I

No.	Name	A	Bx10 <sup>4</sup>	Cx10 <sup>7</sup>	D	Vapor Pressure Range, kPa	Temperature Range, K	ADD <sup>b</sup> %	Number of Data Points	Data Reference Numbers	Calculated Vapor Pressure, kPa, at 400 K
1	Furan	0.858331	-8.56435	9.32123	304.367	0.082-5500.0	193.15-490.25	0.692	62	4, 14, 51	1291.0
2	Cyclobutane	0.870584	-9.76474	19.3674	364.077	0.267-5.760	249.09-298.39	0.786	11	4	362.52
3	2-Tetrahydrofuran	0.830424	-6.81525	7.84786	339.244	1.954-5190.0	233.15-540.15	0.612	67	4, 14, 51	515.10
4	2-Methylfuran	0.871223	-7.95690	7.81737	338.704	86.13-4722.90	233.45-527.61	0.607	32	24, 51	544.33
5	Cyclopentanone	0.897078	-6.60577	4.52567	359.254	643.3-3557.7	427.61-533.72	0.477	20	51	333.02 <sup>c</sup>
6	2-Methyl-2-thiophenol	1.00375	-8.88757	6.83750	428.610	0.324-6132.10	323.20-694.25	1.160	130	2, 4, 6, 11, 16	16.763
7	Phenol	0.833332	-6.42578	7.09855	458.597	274.55-438.92	274.55-438.92	0.372	26	31, 41	45.267
8	Cyclohexanone	0.951396	-8.46102	8.87926	434.658	0.133-101.33	294.15-434.15	1.032	10	41	32.569
9	Cyclohexanol	0.934881	-4.16258	4.00348	400.348	0.133-101.33	280.85-400.65	0.808	10	41	100.03
10	2-Hexanone	0.942238	-10.2065	10.6819	426.827	6.287-67.661	346.49-415.52	0.123	6	16	46.321
11	Benzoic Acid	1.02742	-6.26739	1.92874	479.624	0.266-67.661	340.95-463.65	1.055	18	16	7.4206
12	Anisole	1.01555	-9.95980	7.28734	463.986	0.1238-5010.10	313.20-697.65	0.654	120	4, 6, 12, 16	13.137
13	2-Hydroxytoluene (2-cresol)	0.965085	-6.89845	4.47100	475.222	0.0029-4560.10	278.05-704.85	1.095	110	2, 4, 6, 12, 32, 41	8.3536
14	3-Hydroxytoluene (3-cresol)	1.07944	-11.6938	9.28202	475.109	0.1118-5150.10	323.20-704.85	0.518	123	2, 4, 6, 12, 16	8.4082
15	4-Hydroxytoluene (4-cresol)	0.795901	-4.13024	21.5953	429.907	0.1070-164	273.15-313.15	4.298	7	6	19.856 <sup>c</sup>
16	Coumarone	0.859974	-6.15392	6.99110	474.823	0.133-101.33	310.25-475.55	1.339	48	16, 41	10.259
17	Acetophenone	0.883881	-6.07675	6.44264	480.731	0.133-101.33	319.35-480.65	0.743	29	4, 41	7.7020
18	2-Ethylphenol	0.971667	-6.29566	2.74098	491.415	0.001-133.41	278.11-502.74	1.055	44	4, 15	4.7795
19	3-Ethylphenol	0.979517	-8.35112	6.60684	489.845	0.308-4900.00	343.20-722.95	0.860	110	2, 4, 6, 13, 58	5.4851
20	4-Ethylphenol	0.998991	-8.94506	6.96026	483.876	0.0128-4400.00	298.02-707.95	0.865	120	2, 4, 6, 13, 58	6.5635
21	2,3-Dimethylphenol	0.933879	-8.99374	7.44099	483.942	0.359-4900.00	343.20-707.05	1.175	107	2, 4, 6, 13, 58	6.5604
22	2,4-Dimethylphenol	0.993333	-9.96552	8.34247	474.112	0.1003-4300.00	312.81-701.05	0.6222	109	2, 4, 6, 13, 58	10.348
23	2,5-Dimethylphenol	1.05062	-10.2129	8.04338	499.325	0.265-5000.00	353.20-729.95	0.800	107	2, 4, 6, 13, 58	3.4040
24	3,4-Dimethylphenol	1.04106	-9.50547	6.64831	494.911	0.0901-3600.00	333.20-715.65	0.338	110	2, 4, 6, 13, 58	4.1444
25	3,5-Dimethylphenol	0.881926	-6.65998	7.00344	460.386	0.133-101.33	302.85-460.25	0.554	10	41	15.830
26	2-Ethylanisole	0.874023	-6.87264	7.50986	469.810	0.133-101.33	306.85-469.65	0.620	10	41	12.440
27	3-Ethylanisole	0.872105	-6.70633	7.23277	469.450	0.133-101.33	306.65-469.65	0.700	10	41	12.457
28	4-Ethylanisole	0.913828	-6.36537	7.26448	508.650	0.133-101.33	384.65-506.15	1.128	19	41	2.7081
29	2-Methyl-5-ethylphenol	0.912522	-6.17902	6.51481	487.650	0.133-101.33	329.75-487.65	0.679	10	41	5.2072
30	3-Isopropylphenol	0.901582	-6.42031	6.91585	501.237	0.133-101.33	335.15-501.15	0.738	10	41	3.6502
31	3-Isopropylphenol	0.937791	-6.98550	7.15366	501.658	0.133-101.33	340.15-501.35	0.777	10	41	3.1199
32	3-Phenyl-1-propanol	0.934132	-6.11678	7.13688	508.280	0.133-101.33	347.85-508.15	0.929	10	41	2.2162
33	2-Propylphenol	0.973307	-5.52137	7.84423	494.816	0.666-100.33	414.15-504.65	0.841	16	4	3.7795 <sup>c</sup>
34	4-Propylphenol	0.733568	-5.97977	15.8634	506.614	0.999-100.33	428.35-507.65	1.537	17	4	3.6885
35	2,3,5-Trimethylphenol	0.932985	-5.75276	3.29737	508.477	26.547-133.34	459.63-520.21	0.007	17	4	2.8897 <sup>c</sup>
36	1-Hydroxyethylbenzene	0.881442	-5.80731	6.06214	555.113	0.133-101.33	367.15-555.95	1.181	38	4, 6	0.69877 <sup>c</sup>
37	2-Hydroxyethylbenzene	0.874875	-5.63554	5.87458	560.208	0.667-100.33	401.75-561.15	1.181	27	4, 6	0.61258 <sup>c</sup>
38	2-Ethoxyethylbenzene	0.885386	-5.26451	5.13029	515.194	0.133-101.33	344.55-515.25	0.522	10	41	2.2928
39	4-Ethoxyethylbenzene	0.892200	-6.62186	5.90279	497.209	0.885-104.958	407.80-498.58	0.261	8	41	5.0966 <sup>c</sup>
40	2-Ethoxyethylphenol	0.834403	-6.10916	0.554077	512.690	0.130-133.35	343.15-524.76	1.159	26	4, 41	2.4469
41	4-Ethoxyethylphenol	0.876394	-6.35074	7.65283	521.080	1.333-101.33	387.65-521.15	0.963	19	4	2.2819
42	3-(4-Ethoxyethyl)phenol	0.967228	-6.46894	3.61657	563.562	0.707-103.87	472.47-564.77	0.097	9	4	0.41906 <sup>c</sup>
43	2-(4-Ethoxyethyl)phenol	0.915488	-6.16723	6.81021	505.681	0.133-101.33	343.15-505.75	0.615	10	41	2.6419
44	4-tert-Butyl-2-Cresol	0.894294	-5.55746	5.24049	519.836	0.133-101.33	347.45-520.15	0.530	10	41	1.9869
45	2-Phenylphenol	0.889463	-4.72320	5.27654	549.249	0.133-101.33	373.15-548.15	1.672	28	4, 41	0.53903
46	4-Phenylphenol	0.949514	-5.54686	5.61184	580.171	1.333-101.33	450.15-581.15	0.891	19	4	0.11152 <sup>c</sup>
47	Phenylether	0.893089	-6.11822	7.45086	520.515	0.133-101.33	349.45-520.95	0.914	10	41	1.7438
48	2-tert-Butyl-4-ethylphenol	0.878041	-5.47812	5.36276	536.275	0.133-101.33	361.35-538.45	0.968	10	41	0.93692
49	4-tert-Butyl-2,6-xyleneol	0.871204	-5.99541	9.85796	512.389	0.133-101.33	347.15-512.95	1.513	10	41	1.8914
50	6-tert-Butyl-2,6-xyleneol	0.873072	-6.06053	9.46410	509.117	0.133-101.33	343.45-509.65	1.182	10	41	2.2600
51	6-tert-Butyl-3,4-xyleneol	0.916526	-5.81421	6.69496	522.451	0.133-101.33	357.05-522.65	0.748	10	41	1.2986
52	2,4-Diisopropylphenol	0.916060	-6.48571	5.72246	527.384	0.133-101.33	395.15-528.15	1.665	19	4	1.6685
53	2-Phenylethylphenol	1.23153	-10.1736	637.998	442.318	0.813-18.78	442.35-523.45	1.852	29	4	0.05032 <sup>c</sup>
54	4-Phenylethylphenol	1.25864	-8.45954	-10.7815	664.652	0.560-13.18	447.55-523.65	1.917	23	4	0.02015 <sup>c</sup>

<sup>a</sup> P in atm (1.01325 bar or 101.325 kPa); T in K.

<sup>b</sup> ADD = absolute average deviation.

<sup>c</sup> 400 K outside the temperature range of the data used in evaluating the coefficients of the vapor pressure equation.

Table 18. Coefficients of Vapor Pressure Equation and the Calculated Vapor Pressure at 400 K for More Oxygen Compounds -II

No.	Name	$\log_{10} P = (1-D)/T \times 10 (A + BT + CT^2)^a$				Vapor Pressure Range, kPa	Temperature Range, K	AAD <sup>b</sup> %	No. of Data Points	Data Reference Numbers	Calculated Vapor Pressure, kPa, at 400 K
		A	Bx10 <sup>4</sup>	Cx10 <sup>7</sup>	D						
1	Quinone (p-benzoquinone)	0.902426	-6.04783	6.58278	517.477	0.667-101.33	377.15-518.65	0.864	28	4, 41	1.9583
2	1,2-Dihydroxybenzene	0.958295	-5.78954	5.46841	549.041	0.133-101.33	381.55-549.65	1.358	29	4, 41	0.37720
3	1,3-Dihydroxybenzene	0.941185	-5.32724	5.41185	558.031	1.333-101.33	432.25-559.15	1.150	19	4	0.26743
4	1,4-Dihydroxybenzene	0.935304	-5.45471	6.15169	580.441	1.333-101.33	450.45-582.15	1.664	19	4	0.11370
5	Pyrogallol	0.858892	-4.47192	3.22549	477.010	1.333-101.33	355.15-478.15	2.073	19	4	9.2881
6	Quinalcol										
7	Diphenylene Oxide										
8	Dibenzofuran										
9	2,2'-Di-phenol	0.872661	-6.33808	7.42629	596.940	1.333-101.33	444.15-598.15	0.809	19	4	0.20547
10	Quinhydrone										
11	Anthranthrone										

<sup>a</sup> P in atm (1.01325 bar or 101.325 kPa); T in K.

<sup>b</sup> AAD = absolute average deviation.

<sup>c</sup> 400 K outside the temperature range of the data used in evaluating the coefficients of the vapor pressure equation.

Therefore, the values of *A*, *B*, *C*, and *D* listed in Tables 10-18 may be employed to calculate the  $\Delta H_v$  for the given compounds. In addition, these Cox equations may also be used to extrapolate to either lower or higher temperature regions with reasonable reliability<sup>20</sup> which is the main purpose of this work.

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## 6. References

- "Properties of Hydrocarbons of High Molecular Weight," American Petroleum Institute, Research Project 42, College of Science, The Pennsylvania State University, University Park, Pennsylvania, 1966.
- "Selected Values of Properties of Hydrocarbons and Related Compounds," Thermodynamics Research Center Hydrocarbon Project, Thermodynamics Research Center, Texas A&M University, College Station, Texas (Loose-leaf Data Sheets, Extant, 1982).
- H. C. Anderson and W. R. K. Wu, "Properties of Compounds in Coal-Carbonization Products," Bulletin 606, Bureau of Mines (U.S. GPO, Washington, D.C., 1963).
- T. Boublik, V. Fried, and E. Hala, *The Vapor Pressure of Pure Substances* (Elsevier Scientific, Amsterdam, Netherlands, 1973).
- J. Chao, "Benzene," Key Chemicals Data Books, Thermodynamics Research Center, Texas A&M University, College Station, Texas, 1978.
- "The Coal Tar Data Book," 2nd ed., The Coal Tar Research Association, Oxford Road, Gomersal, Leeds, England, 1965.
- M. P. Doss, "Physical Constants of the Principal Hydrocarbons," 4th ed., Texas, Co., Tech. and Res. Division, New York, New York, 1943.
- Engineering Sciences Data Unit, "Vapor Pressures of Pure Substances Up To Their Critical Points," Vol. 5a-5d, 5f, Engineering Sciences Data Unit, 251-259 Regent Street, London, W1R 7AD, England, 1978.
- W. E. Haines, R. V. Helm, and J. L. Stephens, "Physical Properties of Sulfur Compounds," in Bureau of Mines Bulletin, *Sulfur in Petroleum*, U.S. Bureau of Mines, 1963.
- T. E. Jordan, *Vapor Pressure of Organic Compounds* (Interscience, New York, 1954).
- A. P. Kudchadker, S. A. Kudchadker, and R. C. Wilhoit, "Phenol," Key Chemicals Data Books, Thermodynamics Research Center, Texas A&M University, College Station, Texas, 1977.
- A. P. Kudchadker, S. A. Kudchadker, and R. C. Wilhoit, "Cresols," Key Chemicals Data Books, Thermodynamics Research Center, Texas A&M University, College Station, Texas, 1978.
- A. P. Kudchadker and S. A. Kudchadker, "Xylenols," Key Chemicals Data Books, Thermodynamics Research Center, Texas A&M University, College Station, Texas, 1978.
- A. P. Kudchadker, S. A. Kudchadker, and R. C. Wilhoit, "Furan, Dihydrofuran, Tetrahydrofuran," Key Chemicals Data Books, Thermodynamics Research Center, Texas A&M University, College Station, Texas, 1978.
- O. Shuzo, *Computer Aided Data Book of Vapor Pressures* (Data, Tokyo, Japan, 1976).
- J. Timmermans, *Physico-Chemical Constants of Pure Organic Compounds* (Elsevier, Amsterdam, Netherlands, 1965), Vol. 2.
- N. B. Vargaftik, *Tables on the Thermophysical Properties of Liquids and Gases*, 2nd ed. (Wiley, New York, 1975).
- C. L. Yaws, *Physical Properties* (McGraw-Hill, New York, 1978).
- E. R. Cox, *Ind. Eng. Chem.* **28**, 613 (1936).
- D. W. Scott and A. G. Osborn, *J. Phys. Chem.* **83**, 2714 (1979).
- D. L. Bond and G. Thodos, *J. Chem. Eng. Data* **5**, 289 (1960).
- R. S. Bradley and T. G. Cleasby, *J. Chem. Soc.* 1690 (1953).
- C. G. De Kruif, *J. Chem. Thermodyn.* **12**, 243 (1980).
- C. Eon, C. Pommier, and G. Guiochon, *J. Chem. Eng. Data* **16**, 408 (1971).

- <sup>25</sup>K. A. Kobe and J. F. Mathews, *J. Chem. Eng. Data* **15**, 182 (1970).
- <sup>26</sup>D. Ambrose and C. H. S. Sparke, *J. Chem. Thermodyn.* **8**, 601 (1976).
- <sup>27</sup>T. M. Letcher and F. Marsicano, *J. Chem. Thermodyn.* **6**, 509 (1974).
- <sup>28</sup>A. B. MacKnick and J. M. Prausnitz, *J. Chem. Eng. Data* **24**, 175 (1979).
- <sup>29</sup>D. M. McEachern, O. Sandoval, and J. C. Iniguez, *J. Chem. Thermodyn.* **7**, 299 (1975).
- <sup>30</sup>E. F. Meyer and T. H. Gens, *J. Chem. Eng. Data* **22**, 30 (1977).
- <sup>31</sup>E. F. Meyer and R. D. Hotz, *J. Chem. Eng. Data* **18**, 359 (1973).
- <sup>32</sup>P. Nasir, S. C. Hwang, and R. Kobayashi, *J. Chem. Eng. Data* **25**, 298 (1980).
- <sup>33</sup>D. Ambrose, C. H. S. Sparke, and R. Townsend, *J. Chem. Thermodyn.* **1**, 499 (1969).
- <sup>34</sup>A. G. Osborn and D. R. Douslin, *J. Chem. Eng. Data* **19**, 114 (1974).
- <sup>35</sup>A. G. Osborn and D. R. Douslin, *J. Chem. Eng. Data* **13**, 534 (1968).
- <sup>36</sup>A. G. Osborn and D. R. Douslin, *J. Chem. Eng. Data* **11**, 502 (1966).
- <sup>37</sup>A. G. Osborn and D. W. Scott, *J. Chem. Thermodyn.* **10**, 619 (1978).
- <sup>38</sup>A. G. Osborn and D. R. Douslin, *J. Chem. Eng. Data* **20**, 229 (1975).
- <sup>39</sup>D. W. Scott, W. T. Berg, I. A. Hossenlopp, W. N. Hubbard, J. F. Messerly, S. S. Tood, D. R. Douslin, J. P. McCullough, and G. Waddington, *J. Phys. Chem.* **71**, 2263 (1967).
- <sup>40</sup>R. K. Sharma and J. B. Palmer, *J. Chem. Eng. Data* **19**, 6 (1974).
- <sup>41</sup>D. R. Stull, *Ind. Eng. Chem.* **39**, 517 (1947).
- <sup>42</sup>C. Van De Rostyne and J. M. Prausnitz, *J. Chem. Eng. Data* **25**, 1 (1980).
- <sup>43</sup>P. T. White, D. G. Barnard-Smith, and F. A. Filder, *Ind. Eng. Chem.* **144**, 1430 (1952).
- <sup>44</sup>S. A. Wiczorek and R. Kobayashi, *J. Chem. Eng. Data* **25**, 302 (1980).
- <sup>45</sup>D. Ambrose, I. J. Lawrenson, and C. H. S. Sparke, *J. Chem. Thermodyn.* **7**, 1173 (1975).
- <sup>46</sup>A. J. B. Cruickshank and A. J. B. Cuttler, *J. Chem. Eng. Data* **12**, 326 (1967).
- <sup>47</sup>J. A. Hugill and M. L. McGlashan, *J. Chem. Thermodyn.* **10**, 95 (1978).
- <sup>48</sup>D. Ambrose, I. J. Lawrenson, and C. H. S. Sparke, *J. Chem. Thermodyn.* **8**, 503 (1976).
- <sup>49</sup>D. W. Morecroft, *J. Chem. Eng. Data* **9**, 488 (1964).
- <sup>50</sup>G. J. Pasek and G. Thodos, *J. Chem. Eng. Data* **7**, 21 (1962).
- <sup>51</sup>K. A. Kobe, A. E. Ravicz, and S. P. Vohra, *J. Chem. Eng. Data* **1**, 50 (1956).
- <sup>52</sup>E. B. Munday, J. C. Mullins, and D. D. Edle, *J. Chem. Eng. Data* **25**, 191 (1980).
- <sup>53</sup>S. A. Wiczorek and R. Kobayashi, *J. Chem. Eng. Data* **26**, 8 (1980).
- <sup>54</sup>D. C. K. Lin, H. Silberberg, and J. J. McKetta, *J. Chem. Eng. Data* **15**, 483 (1970).
- <sup>55</sup>D. Ambrose, B. E. Broderick, and R. Townsend, *J. Chem. Soc. (A)*, 633 (1967).
- <sup>56</sup>A. G. Osborn and D. W. Scott, *J. Chem. Thermodyn.* **12**, 429 (1980).
- <sup>57</sup>N. K. Smith, R. C. Stewart, Jr., A. G. Osborn, and D. W. Scott, *J. Chem. Thermodyn.* **12**, 919 (1980).
- <sup>58</sup>R. J. L. Andon, D. P. Biddiscombe, J. D. Cox, R. Handley, D. Harrop, E. F. G. Herington, and J. F. Martin, *J. Chem. Soc.* 5246 (1960).
- <sup>59</sup>G. Bardi, R. Gigli, L. Malaspina, and V. Piacente, *J. Chem. Eng. Data* **18**, 127 (1973).
- <sup>60</sup>L. M. Besley and G. A. Bottomley, *J. Chem. Thermodyn.* **6**, 577 (1974).
- <sup>61</sup>B. Stevens, *J. Chem. Soc.*, 2973 (1953).
- <sup>62</sup>J. J. Murray, R. F. Pottie, and C. Pupp, *Can. J. Chem.* **52**, 557 (1974).
- <sup>63</sup>H. Inokuchi, S. Shiba, T. Honda, and H. Akamatu, *J. Chem. Soc. Jpn.* **73**, 299 (1952).
- <sup>64</sup>S. H. Lee-Bechtold, I. A. Hossenlopp, D. W. Scott, A. G. Osborn, and W. D. Good, *J. Chem. Thermodyn.* **11**, 469 (1979).
- <sup>65</sup>H. Hoyer and W. Peperle, *Z. Elektrochem.* **62**, 61 (1958).
- <sup>66</sup>O. A. Nelson and H. Wales, *J. Am. Chem. Soc.* **47**, 867 (1925).
- <sup>67</sup>J. F. T. Berliner and O. E. May, *J. Am. Chem. Soc.* **49**, 1007 (1927).
- <sup>68</sup>E. A. Coulson and J. I. Jones, *J. Soc. Chem. Ind. London* **65**, 169 (1946).
- <sup>69</sup>G. E. Williams and E. C. Gilbert, *J. Am. Chem. Soc.* **64**, 2776 (1942).
- <sup>70</sup>G. B. Heisig, *J. Am. Chem. Soc.* **63**, 1698 (1941).
- <sup>71</sup>M. W. Lister, *J. Am. Chem. Soc.* **63**, 143 (1941).
- <sup>72</sup>J. Chipman and S. B. Peltier, *Ind. Eng. Chem.* **21**, 1106 (1929).
- <sup>73</sup>G. M. Wilson, R. H. Johnston, S. C. Hwang, and C. Tsouopoulos, *Ind. Eng. Chem., Process Des. Dev.* **20**, 94 (1981).
- <sup>74</sup>P. Nasir, A. Sivaraman, and R. Kobayashi, "An Integrated Experimental Computational Approach to Evaluate the Fugacity Function of Dibenzofuran at High Temperature and Pressures" (private communication, 1982).
- <sup>75</sup>A. Sivaraman and R. Kobayashi, "Investigation of Vapor Pressures and Heat of Vaporization of Condensed Heterocyclic Aromatic Compounds at Elevated Temperature" (private communication, 1982).
- <sup>76</sup>W. Wagner, *Cryogenics* **8**, 470 (1973).
- <sup>77</sup>G. Raam Somayajulu (private communication).
- <sup>78</sup>L. Borrelli, J. Holste, T. Eubank, and K. R. Hall, "A Concise Description of the Saturation Properties," presented at National AIChE Meeting, Orlando, Florida, March 1982.
- <sup>79</sup>J. D. Cox and G. Pilcher, *Thermochemistry of Organic and Organometallic Compounds* (Academic, New York, 1970), p. 105.