

Vapor Pressure of Coal Chemicals

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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-

mited 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,² 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,³ the vapor pressure data on many classes of chemical substances were represented by Chebyshev equations.

Recently, the Wagner equation⁷⁶ 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 equations¹⁹ for presenting the vapor pressure data on hydrocarbons,³⁴ nitrogen compounds,³⁵ and sulfur compounds³⁶ 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 Osborn²⁰ 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 Somayajulu⁷⁷ and Borrelli *et al.*⁷⁸ 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.^{2,4,6,8,16,35,41,62,65}

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 I. Vapor pressure data on benzene and its derivatives

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

No.	Formula	Name	Vapor Pressure Range, kPa ^a	Temperature Range, K	Number of Data Points	Reference Number	Authors	Year Published	Data Types and Method of Measurement ^b	References Citing the Same Data
28	C ₁₀ H ₁₄	1-Methyl-4-isopropylbenzene	1.393 ~ 200.6 12.026 ~ 104.55 0.121 ~ 2694.2	330.3 ~ 480.3 380.19 ~ 451.57 290. ~ 650.	55 7 73	2 4 8	TICHP Boublik, T. et al. Eng. Sci. Data Unit	1978 1973 1978	C B C	15
29	C ₁₀ H ₁₄	1,2-Diethylbenzene	1.331 ~ 198.2 6.425 ~ 104.02 0.112 ~ 2901.5	335.9 ~ 485.9 298.75 ~ 449.65 295. ~ 660.	55 20 74	2 4 8	TICHP Boublik, T. et al. Stull, D.R.	1978 1973 1947	C B C	10 15, 16
30	C ₁₀ H ₁₄	1,3-Diethylbenzene	1.427 ~ 197.3 6.423 ~ 104.02 0.119 ~ 2716.8	335.9 ~ 483.1 368.242 ~ 455.31 295. ~ 650.	54 20 72	2 4 8	TICHP Boublik, T. et al. Stull, D.R.	1978 1973 1947	C B C	10 15, 16
31	C ₁₀ H ₁₄	1,4-Diethylbenzene	0.133 ~ 101.33 1.331 ~ 196.6 0.122 ~ 161.02	335.9 ~ 485.9 329. ~ 455.35 335.9 ~ 457.97	55 20 73	2 4 8	TICHP Boublik, T. et al. Eng. Sci. Data Unit	1978 1973 1947	C B C	10 15, 16
32	C ₁₀ H ₁₄	1,2-Dimethyl-3-ethylbenzene	1.331 ~ 199.98 0.139 ~ 2956.5	344.25 ~ 497.15 305. ~ 675.	27 75	2 8	TICHP Eng. Sci. Data Unit	1978 1978	C C	10
33	C ₁₀ H ₁₄	1,2-Dimethyl-4-ethylbenzene	1.331 ~ 199.98 0.114 ~ 2858.4	341.05 ~ 492.85 300. ~ 665.	27 74	2 8	TICHP Eng. Sci. Data Unit	1978 1978	C C	
34	C ₁₀ H ₁₄	1,3-Dimethyl-2-ethylbenzene	1.358 ~ 204.8	341.4 ~ 494.2	56	2	TICHP	1978	C	
			0.112 ~ 2964.6	300. ~ 670.	75	8	Eng. Sci. Data Unit	1978	C	
35	C ₁₀ H ₁₄	1,3-Dimethyl-4-ethylbenzene	1.269 ~ 199.9 0.130 ~ 2852.5	388.7 ~ 491.4 300. ~ 665.	56 74	2 8	TICHP Eng. Sci. Data Unit	1978 1978	C C	
36	C ₁₀ H ₁₄	1,3-Dimethyl-5-ethylbenzene	0.133 ~ 101.33 1.310 ~ 197.2	296.35 ~ 457.65 335.9 ~ 485.9	10 55	41 2	TICHP Eng. Sci. Data Unit	1947 1978	C C	
37	C ₁₀ H ₁₄	1,4-Dimetyl-2-ethylbenzene	0.107 ~ 2631.3 0.133 ~ 101.33	295. ~ 650. 296.35 ~ 458.15	72 10	8 41	TICHP Eng. Sci. Data Unit	1978 1947	C C	
38	C ₁₀ H ₁₄	1,2,3,4-Tetramethylbenzene	0.133 ~ 101.33 1.289 ~ 101.33	338.7 ~ 488.7 297.25 ~ 458.15	78 10	8 41	TICHP Eng. Sci. Data Unit	1978 1947	C C	
39	C ₁₀ H ₁₄	1,2,3,5-Tetramethylbenzene	0.3401 ~ 107.31 1.289 ~ 204.8	330. ~ 480. 347.0 ~ 502.6	16 57	10 8	TICHP Eng. Sci. Data Unit	1954 1978	C C	
40	C ₁₀ H ₁₄	1,2,4,5-Tetramethylbenzene	0.106 ~ 2850.3 0.3988 ~ 98.765	305. ~ 675. 330. ~ 470.	75 15	6 2	TICHP Eng. Sci. Data Unit	1978 1978	C C	
41	C ₁₁ H ₁₆	sec-Amylbenzene	1.351 ~ 198.6 0.133 ~ 101.33	347.0 ~ 499.8 300. ~ 470.	56 15	8 10	Eng. Sci. Data Unit Jordan, T.E.	1978 1954	C C	10, 15
42	C ₁₁ H ₁₆	3-Ethyl-1-isopropylbenzene	0.133 ~ 101.33	301.45 ~ 466.15	10	41	Stull, D.R.	1947	C	10, 15
43	C ₁₁ H ₁₆	4-Ethyl-1-isopropylbenzene	0.133 ~ 101.33	304.65 ~ 468.95	10	41	Stull, D.R.	1947	C	10, 15
44	C ₁₁ H ₁₆	3,5-Diethyltoluene	0.133 ~ 101.33	304.95 ~ 472.15	10	41	Stull, D.R.	1947	C	15
45	C ₁₁ H ₁₆	1,2,4-Trimethyl-5-ethylbenzene	1.467 ~ 9.466 0.133 ~ 101.33	360.45 ~ 405.5 316.85 ~ 481.25	11 10	4 41	Boublik, T. et al. Stull, D.R.	1973 1947	C C	15
46	C ₁₁ H ₁₆	2,5-Trimethyl-2-ethylbenzene	1.573 ~ 101.33	361.65 ~ 483.35	19	41	Boublik, T. et al. Stull, D.R.	1973 1947	C C	
47	C ₁₂ H ₁₈	1,2-Diisopropylbenzene	0.133 ~ 101.33	311.95 ~ 481.15	10	41	Boublik, T. et al. Stull, D.R.	1973 1947	B C	15 10, 15
48	C ₁₂ H ₁₈	1,3-Diisopropylbenzene	0.133 ~ 101.33	307.85 ~ 475.15	10	41	Stull, D.R.	1947	C	10, 15
49	C ₁₂ H ₁₈	1,4-Diisopropylbenzene	6.753 ~ 104.63	393.41 ~ 484.73	7	4	Boublik, T. et al.	1973	B	15
50	C ₁₂ H ₁₈	1,2,4-Triethylbenzene	0.133 ~ 101.33	319.15 ~ 491.15	10	41	Stull, D.R.	1947	C	10, 15
51	C ₁₂ H ₁₈	1,3,4-Triethylbenzene	0.133 ~ 101.33	321.05 ~ 490.65	10	41	Stull, D.	1947	C	
52	C ₁₂ H ₁₈	Mexamethylbenzene	2.80 x 10 ⁻⁷ ~ 0.014	303.10 ~ 343.02	9	43	Ambrose, D.	1976	A, static	

^a 1 kPa = 7.50062 torr (mm Hg)^b

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

a 1 kPa = 7.5002 torr (mm Hg).

$b = 7.5002 \text{ torr (mm Hg)}$.

A = experimental data measured by the author(s) of the reference.

B = experimental data collected from literature by the author(s) of the references

C = calculated values from a regression.

Table 3. Vapor pressure data on saturated ring compounds

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

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

No.	Formula	Name	Vapor Pressure Range, kPa ^a	Temperature Range, K	Number of Data Points	Reference Number	Authors	Year Published	Data Types ^b and Method of Measurement	Reference Citing the Same Data
7	C ₇ H ₁₄	Cycloheptane	1.333-199.98 19.920-270.111	284.35-418.88 341.354-432.172	27 15	2 4	TRCHP Boublík, T. et al	1978 1973	C B	15
8	C ₇ H ₁₄	Ethylcyclopentane	1.333-199.98 6.41-103.99 1.341-3143. 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 Boublík, T. et al Vargaftik, N. B. Stull, D. R.	1978 1973 1975 1947	C B B C	10 10,15
9	C ₇ H ₁₄	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 Boublík, T. et al Vargaftik, N. B.	1978 1973 1975	C B B	10 3,15
10	C ₇ H ₁₄	1,cis-2-Dimethylcyclopentane	1.333-199.98 6.41-103.99	271.89-398.35 298.457-379.596	27 20	2 4	TRCHP Boublík, T. et al	1978 1973	C B	10 15
11	C ₇ H ₁₄	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 Boublík, T. et al	1978 1973	C B	10 15
12	C ₇ H ₁₄	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 Boublík, T. et al	1978 1973	C B	10 15
13	C ₇ H ₁₄	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 Boublík, T. et al	1978 1973	C B	10 15
14	C ₇ H ₁₄	Methylcyclohexane	1.333-199.98 6.35-103.92 1.333-199.98 0.0036-3116.0	269.55-400.15 298.736-374.982 269.95-400.15 203.2-563.2	27 20 30 38	2 4 6 17	TRCHP Boublík, T. et al Coal Tar Res. Ass. Vargaftik, N. B.	1978 1973 1965 1975	C B B B	10 10
15	C ₈ H ₁₆	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 ₈ H ₁₆	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 Boublík, 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 ^a	Temperature Range, K	Number of Data Points	Reference Number	Authors	Year Published	Data Types ^b and Method of Measurement	Reference Citing the Same Data
17	C ₈ H ₁₆	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 ₈ H ₁₆	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 ₈ H ₁₆	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 ₈ H ₁₆	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 ₈ H ₁₆	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 ₈ H ₁₆	1,trans-4-Di-methylcyclohexane	1.333-199.98 0.133-101.33	283.2-420.0 248.9-392.5	27 10	2 41	TRCHP Stull, D. R.	1978 1947	C C	
23	C ₈ H ₁₆	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 ₈ H ₁₆	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 ₈ H ₁₆	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 ₈ H ₁₆	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 ₈ H ₁₆	1,1,2-Trimethylcyclopentane	6.41-104.00 1.333-199.98	309.357-387.836 279.53-413.75	19 27	4 2	Boublik, T. et al TRCHP	1973 1978	B C	15
28	C ₈ H ₁₆	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 ^a	Temperature Range, K	Number of Data Points	Reference Number	Authors	Year Published	Data Types ^b and Method of Measurement	Reference Citing the Same Data
29	C ₉ H ₁₈	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 ₉ H ₁₈	Isopropylcyclohexane	6.411-104.01	343.665-428.752	20	4	Boublik, T. et al	1973	B	
31	C ₉ H ₁₈	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 ₉ H ₁₈	1,1,3 - Trimethylcyclohexane	6.398-104.00	327.819-410.786	20	4	Boublik, T. et al	1973	B	50
33	C ₁₀ H ₂₀	n-Butylcyclohexane	1.333-199.98	332.65-484.35	27	2	TRCHP		C	
34	C ₁₀ H ₂₀	Isobutylcyclohexane	6.41-104.01	357.902-445.544	20	4	Boublik, T. et al	1973	B	8
35	C ₁₀ H ₂₀	sec-Butylcyclohexane	6.41-104.01	367.608-453.571	20	4	Boublik, T. et al	1973	B	
36	C ₁₀ H ₂₀	tert-Butylcyclohexane	6.40-104.00	357.183-445.820	20	4	Boublik, T. et al	1973	B	

^a 1 kPa = 7.50062 torr (mmHg)^b 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 ^a	Temperature Range, K	Number of Data Points	Reference Number	Authors	Year Published	Data Types ^b and Method of Measurement	Reference Citing the Same Data
1	C ₄ H ₆	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 ₅ H ₆	1,3-Cyclopentadiene	18.821-96.327	271.25-313.05	6	15	Shuzo, O.	1978	B	
3	C ₅ H ₈	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 ₆ H ₈	1,3-Cyclohexdiene	16.8-34.76 307.34-363.31	303.96-322.03 19,444-135.198	7 12	27 31	Letcher,T.M. et al Meyer, E. F. et al	1974 1973	A, Static A Ebullionmetric	15
5	C ₆ H ₈	1,4-Cyclohexdiene	11.89-25.25	304.25-322.23	7	27	Letcher,T.M. et al	1974	A, Static	
6	C ₆ H ₁₀	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, Ebullionmetric A, Static	15
7	C ₉ H ₈	Indene	0.133-104.41 0.133-101.33	289.55-456.97 289.6-454.8	10 10	16 41	Coal Tar Res. Ass. Stull, D. R.	1965 1947	B C	10
8	C ₉ H ₁₀	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 ₁₀ H ₁₂	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 ₁₀ H ₁₈	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 ^a	Temperature Range, K	Number of Data Points	Reference Number	Authors	Year Published	Data Types ^b and Method of Measurement	Reference Citing the Same Data
11	C ₁₀ H ₁₈	trans-Decalin	2.666-13.333 5.53-102.73 0.133-101.33	346.15-390.15 365.510-461.017 272.35-459.85	5 19 10	1 4 41	API 42 Boublik, T. et al Stull, D. R.	1966 1973 1947	A B C	
12	C ₁₁ H ₁₄	1,1-Dimethylindan	0.258-101.325	313.15-467.22	24	37	Osborn, A.G. et al	1978	A, Ebulliometric	
13	C ₁₁ H ₁₄	4,6-Dimethylindan	0.057-47.38	313.15-467.22	18	37	Osborn, A.G. et al	1978	A, Ebulliometric	
14	C ₁₁ H ₁₄	4,7-Dimethylindan	0.050-47.375	313.15-469.97	17	37	Osborn, A.G. et al	1978	A, Ebulliometric	
15	C ₁₂ H ₈	Biphenylene	0.0176-1.8352	338.15-408.15	16	56	Osborn, A.G. et al	1980	A, Static	
16	C ₁₂ H ₁₀	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. Vargaftik, 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, Isotenlsopic	
17	C ₁₂ H ₁₆	Phenylcyclohexane	264.8-2457.3	560.93-727.59	7	73	Wilson, G.M. et al	1981	A, Static	
18	C ₁₂ H ₂₂	Bicyclohexyl	9.59-346.69 0.067-1.333	424.25-577.25 321.15-376.15	23 5	44 1	Wieczorek, S.A. et al API 42	1980 1966	A, Static A	
19	C ₁₂ H ₂₂	1,1-Dicyclo-pentylethane	0.067-1.333	385.65-430.65	5	1	API 42	1966	A,	
20	C ₁₃ H ₁₂	Biphenylmethane	0.067-1.333 32.33-146.89 0.133-101.33 390-670.12 15.93-1827.1	343.2-400.2 490.69-555.39 349.15-537.65 424.64-647.25 560.93-727.59	5 9 10 32 7	1 16 41 44 73	API 42 Timmermans, J. Stull, D. R. Wieczorek, S.A. et al Wilson, G. M. et al	1966 1965 1947 1980 1981	A, B C A, Static A, Static	
21	C ₁₃ H ₁₈	1,1,4,6-Tetra-methylindan	0.032-38.565	313.15-468.64	18	37	Osborn, A. G. et al	1978	A, Ebulliometric	
22	C ₁₃ H ₁₈	1,1,4,7-Tetra-methylindan	0.025-31.177	313.15-468.80	18	37	Osborn, A. G. et al	1978	A, Ebulliometric	

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

No.	Formula	Name	Vapor Pressure Range, kPa ^a	Temperature Range, K	Number of Data Points	Reference Number	Authors	Year Published	Data Types ^b and Method of Measurement	Reference Citing the Same Data
23	C ₁₄ H ₁₂	Biphenylethylene	0.067-1.333	350.15-407.15	5	1	API 42	1966	A,	
24	C ₁₄ H ₁₄	1,1-Diphenylethane	0.067-1.333	348.65-404.65	5	1	API 42	1966	A,	
25	C ₁₄ H ₁₄	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 ₁₄ H ₂₀	2-Butyltetralin	0.067-1.333	354.65-410.65	5	1	API 42	1966	A,	
27	C ₁₄ H ₂₀	1-Cyclohexyl-1-phenylethane	0.067-1.333	345.15-399.65	5	1	API 42	1966	A,	
28	C ₁₄ H ₂₀	2-Cyclohexyl-1-phenylethane	0.067-1.333	348.15-406.15	5	1	API 42	1966	A,	
29	C ₁₄ H ₂₀	3-Cyclopentyl-1-phenylpropane	0.067-1.333	348.15-406.15	5	1	API 42	1966	A,	
30	C ₁₄ H ₂₆	1,1-Dicyclohexyl-ethane	0.067-1.333	346.15-402.15	5	1	API 42	1966	A,	
31	C ₁₄ H ₂₆	1,2-Dicyclohexyl-ethane	0.067-1.333	347.65-402.15	5	1	API 42	1966	A,	

^a 1 kPa = 7.50062 torr (mmHg)^b A = Experimental Data Measured by the Authors(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 ^a	Temperature Range, K	Number of Data Points	Reference Number	Authors	Year Published	Data Types ^b and Method of Measurement	Reference Citing the Same Data
1	C ₂ H ₄ 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 ₃ H ₆ 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 ₄ H ₄ 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 ₄ H ₈ S	Tetrahydrothiophene	12.95-54.93 1.333-199.98	333.45-373.45 287.35-420.609	5 27	24 2	Eon, C. et al TRCHP	1971 1978	A, Isoteniscopic C	15
5	C ₄ H ₈ S	Thiacyclopentane	1.333-199.98 19.920-270.111 11.67-122.51	287.38-420.61 344.332-433.601 331.31-401.56	27 15 19	2 36 43	TRCHP Osborn,A.G. et al White, P.T. et al	1978 1966 1952	C A, Static & Ebulliometric A, Ebulliometric	4,15,16
6	C ₅ H ₆ 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 ₅ H ₆ 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 ₅ H ₁₀ S	Cyclopentanethiol	19.920-270.111	354.024-445.933	15	38	Osborn,A.G. et al	1966	A,State & Ebulliometric	4
9	C ₅ H ₁₀ 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 ^a	Temperature Range, K	Number of Data Points	Reference Number	Authors	Year Published	Data Types ^b and Method of Measurement	Reference Citing the Same Data
10	C ₅ H ₁₀ S	3-Methylthiacyclopentane	1.333-199.98 9.582-270.111 11.68-133.03	300.25-439.026 340.690-452.626 345.71-422.38	27 21 20	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
11	C ₅ H ₁₀ S	Thiacyclohexane	1.333-199.98 13.332-101.33 11.65-129.10	302.35-443.15 351.43-414.90 348.01-422.16	27 5 17	2 4 43	TRCHP Boublik, T. et al White, P.T. et al	1978 1973 1952	C B A, Ebulliometric	15 9
12	C ₆ H ₁₀ S	Benzenthiol	1.333-199.98 19.920-270.111 0.133-101.33 2.000-101.33	325.43-471.102 387.693-485.310 291.75-441.15 339.15-441.15	27 15 10 9	2 36 41 9	TRCHP Osborn, A.G. et al Stull, D.R. Haines, W.E. et al	1978 1966 1947 1963	C A, Static & Ebulliometric C B	4, 15
13	C ₆ H ₈ S	2,5-Dimethylthiaphene	7.40-34.26	333.45-373.45	5	24	Eon, C. et al	1971	A, Isoteniscopic	
14	C ₆ H ₈ S	2-Ethylthiophene	8.12-37.33	333.45-373.45	5	24	Eon, C. et al	1971	A, Isoteniscopic	
15	C ₆ H ₁₂ S	Cyclohexanethiol	9.582-270.111 1.60-101.32	356.89-475.80 314.15-431.15	21 6	36 9	Osborn, A.G. et al Haines, W.E. et al	1966 1963	A, Static & Ebulliometric	4, 15
16	C ₆ H ₁₂ S	2,cis-5-Dimethyl-thiacyclopentane	1.333-199.98 11.65-133.01	303.15-444.15 348.86-426.37	27 19	2 43	TRCHP White, P.T. et al	1978 1952	C A, Ebulliometric	9
17	C ₆ H ₁₂ S	2,trans-5-Dimethyl-thiacyclopentane	1.333-199.98 11.65-59.39	302.15-443.15 348.05-395.82	27 13	2 43	TRCHP White, P.T. et al	1978 1952	C A, Ebulliometric	9
18	C ₆ H ₁₂ S	2-Methylthiacyclohexane	1.333-199.98 11.65-133.10	309.15-455.15 356.84-437.32	30 20	2 43	TRCHP White, P.T. et al	1978 1952	C A, Ebulliometric	9
19	C ₆ H ₁₂ S	3-Methylthiacyclohexane	1.333-199.98 11.65-91.59	313.15-460.15 361.23-427.18	30 15	2 43	TRCHP White, P.T. et al	1978 1952	C A, Ebulliometric	9
20	C ₆ H ₁₂ S	4-Methylthiacyclohexane	1.333-199.98 11.65-122.01	314.15-461.15 361.66-439.37	30 19	2 43	TRCHP White, P.T. et al	1978 1952	C A, Ebulliometric	9

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

No.	Formula	Name	Vapor Pressure Range, kPa ^a	Temperature Range, K	Number of Data Points	Reference Number	Authors	Year Published	Data Method	Types ^b and Band C	Reference Citing the Same Data
21	C ₇ H ₈ S	2-Methylbenzenthiol	1.333-199.98	343.15-498.15	27	2	TRCHP	1978	C		
22	C ₇ H ₈ S	3-Methylbenzenthiol	1.333-199.98	345.15-498.15	27	2	TRCHP	1978	C		
23	C ₇ H ₈ S	4-Methylbenzenthiol	1.333-199.98	343.15-499.15	27	2	TRCHP	1978	C		
24	C ₇ H ₈ 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, W.E. et al	1966 1963	A, Static & Ebulliometric. B	4	
25	C ₁₀ H ₈ S	1-Naphthalenethiol	0.200-101.33	379.15-559.15	8	9	Haines, W.E. et al	1963	B		
26	C ₁₀ H ₈ S	2-Naphthalenethiol	1.373-101.33	419.45-559.15	6	9	Haines, W.E. et al	1963	B		
27	C ₁₂ H ₈ S	Dibenzothiophene	0.471-105.902	424.81-607.53	19	75	Sivaraman, A. et al	1982	A, Static		
28	C ₁₂ H ₈ S	Diphenylthiomethane	0.00267-101.33	368.2-569.2	17	9	Haines, W.E. et al	1963	B		

^a 1 kPa = 7.50062 torr (mmHg)^b 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

No.	Formula	Name	Vapor Pressure Range, kPa ^a	Temperature Range, K	Number of Data Points	Reference	Authors	Year Published	Data Types, Methods of Measurement ^b	Reference Citing the Same Data Set
1	C ₂ H ₅ N	Aziridine	0.001-9363.2	175-520.	70	8	Eng. Sci. Data Unit	1978	C	
2	C ₃ H ₇ N	Azetidine	0.001-8539.7	180-545.	74	8	Eng. Sci. Data Unit	1978	C	
3	C ₄ H ₉ N	Pyrrole	0.021-6832.3 8.39-42.26 9.582-270.11 359.-2034.	250.-635. 333.5-371.5 338.82-439.26 450.-544.	78 5 21 18	8 24 35 51	Eng. Sci. Data Unit Eon, C., et al. Osborn, A.G., et al. Kobe, K.A., et al. Eng. Sci. Data Unit	1978 1971 1968 1956 1968	C A, Isoteniscopic A, Static & Ebul. A, Static A, Static & Ebul. C	15 4, 15, 39 6 4, 15
4	C ₄ H ₉ N	Pyrrolidine	0.014-5399.1 19.920-270.11 0.121-270.11 0.029-5645.0	215.-565. 19.920-270.11 340.440-426.036 253.-426.04	15 27 71 78	8 24 35 6	Eng. Sci. Data Unit Osborn, A.G., et al. Coal Tar Res. Ass. Eng. Sci. Data Unit	1978 1956 1965 1978	C A, Static & Ebul. B C	4, 15 10
5	C ₅ H ₁₁ N	Pyridine	8.506-101.98 462.-5433. 0.016-4790.5	320.477-388.623 450.-617 320.-395	22 31 74	16 51 8	Timmermans, J. Kobe, K.A., et al. Eng. Sci. Data Unit	1965 1956 1978	B A, Static	
6	C ₅ H ₁₁ N	1-Methylpyrrole	0.022-32.5	320.477-388.623	5	24	Eng. Sci. Data Unit Osborn, A.G., et al. Eng. Sci. Data Unit	1978 1956 1978	C A, Isoteniscopic	15
7	C ₅ H ₁₁ N	Piperidine	9.582-270.11 3.04-101. 9.580-270.07 0.667-101.3	222.112-322.590 292.65-379.49 315.511-416.763 266.2-426.0	21 32 21 9	35 16 35 41	Eng. Sci. Data Unit Timmermans, J. Osborn, A.G., et al. Boeblik, T., et al.	1978 1965 1968 1947	C A, Static & Ebul. B C	4, 15
8	C ₆ H ₇ N	Aniline	6.807-104.59 0.008-2165.7 6.786-101.8 0.133-2900.0	375.747-458.30 262.1-457.2 375.95-457.60 300.0-699.2	7 86 46 19	4 8 16 41	Eng. Sci. Data Unit Osborn, A.G., et al. Timmermans, J. Vargashik, M.D.	1965 1965 1965 1975	B C B C	10
9	C ₆ H ₇ N	2-Methylpyridine	0.133-101.3 2.67-5281.83 9.920-270.11 0.001-4388.7	308.0-457.6 350.55-699.15 322.944-430.506 265.-590	19 13 15 66	35 16 35 8	Taylor, C.L., et al. Osborn, A.G., et al. Coal Tar Res. Ass. Eng. Sci. Data Unit	1978 1968 1965 1978	C A, Static & Ebul. B C	4, 15, 16
10	C ₆ H ₇ N	3-Methylpyridine	9.582-270.11 16.31-101.1 9.035-400.0	347.186-457.718 369.-417.1 255.-457.60	22 12 84	68 68 35	Stull, D.R., et al. Coulson, E.A., et al. Osborn, A.G., et al. Eng. Sci. Data Unit	1947 1946 1968 1978	C A, Lateniscopic A, Static & Ebul.	10 4, 6, 15, 16
11	C ₆ H ₇ N	4-Methylpyridine	0.133-101.3 0.234-4586.2 10.35-101.59	359.8-432.251 280.-645. 350.056-418.612	20 74 21	16 8 16	Timmermans, J. Osborn, A.G., et al. Eng. Sci. Data Unit	1965 1968 1978	B C B	4, 15
12	C ₆ H ₈ N	2,5-Dimethylpyrrole	9.582-270.11	348.202-459.085	62	35	Eng. Sci. Data Unit	1978	A, Static & Ebul.	4, 6, 15, 16
13	C ₆ H ₁₁ N	Cyclohexylamine	9.582-232.09	373.710-472.389	15	16	Osborn, A.G., et al. Timmermans, J.	1968 1965	A, Static & Ebul. B	4 15
14	C ₆ H ₁₁ N	2-Methylpiperidine	0.443-3666.3	270.-595.	66	8	Eng. Sci. Data Unit	1978	C	
15	C ₇ H ₉ N	Benzylamine	9.582-270.11 0.001-4745.4 0.133-101.3	324.630-430.679 250.-685. 302.2-457.6	21 68 10	35 41	Osborn, A.G., et al. Eng. Sci. Data Unit Stull, D.R.	1968 1978 1947	A, Static & Ebul. C C	4, 15
16	C ₇ H ₉ N	2-Ethylpyridine	0.001-3908.2	220.-630.	83	8	Eng. Sci. Data Unit	1978	C	
17	C ₇ H ₉ N	3-Ethylpyridine	0.001-3955.2	225.-660.	88	8	Eng. Sci. Data Unit	1978	C	
18	C ₇ H ₉ N	4-Ethylpyridine	0.001-3962.8	230.-660.	87	8	Eng. Sci. Data Unit	1978	C	
19	C ₇ H ₉ N	2,3-Dimethylpyridine	0.010-4086.3 14.583-104.70	260.-655. 372.693-435.562	80 22	8 16	Eng. Sci. Data Unit Timmermans, J.	1978 1965	C B	4
20	C ₇ H ₉ N	2,4-Dimethylpyridine	2.37-6 0.025-3862.5	325.-7344.7 260.-645.	2 78	6 8	Coal Tar Res. Ass. Eng. Sci. Data Unit	1965 1978	B C	
21	C ₇ H ₉ N	2,5-Dimethylpyridine	6.237-105.18 0.026-3886.8	349.396-432.975 260.-640.	77	16	Eng. Sci. Data Unit Timmermans, J.	1965 1978	C B	4, 15
22	C ₇ H ₉ N	2,6-Dimethylpyridine	0.108-721.5 13.607-102.02	352.447-430.49 352.447-417.45	71 24	16 16	Eng. Sci. Data Unit Timmermans, J.	1978 1965	C B	4, 15
23	C ₇ H ₉ N	3,4-Dimethylpyridine	18.89-100.7 86.880-104.46	319.2-417.0 446.254-453.499	10 12	68 4	Coulson, E.A., et al. Boeblik, T., et al.	1946 1973	A, Isoteniscopic B C	4, 6, 15
24	C ₇ H ₉ N	3,5-Dimethylpyridine	79.928-103.46	436.000-445.879	81	14	Eng. Sci. Data Unit Boeblik, T., et al.	1973	B C	15
25	C ₇ H ₉ N	N-Methylaniline	0.452-11.28	125.-157.-72.76	26	4	Eng. Sci. Data Unit Boeblik, T., et al.	1973	B	
26	C ₇ H ₉ N	2-Methylaniline	0.001-4693.7 7.605-101.33	255.-700. 391.61-473.45	80 7	41 8	Eng. Sci. Data Unit Stull, D.R.	1978 1947	B C	
27	C ₇ H ₉ N	3-Methylaniline	0.133-6.67 7.605-101.33	319.4-388.3 315.-73.	50 91	9 9	Eng. Sci. Data Unit Boeblik, T., et al.	1965 1973	B C	6, 15, 16
28	C ₇ H ₉ N	4-Methylaniline	0.001-4443.4	320.1-473.6	65	8	Eng. Sci. Data Unit Boeblik, T., et al.	1973	B C	16
29	C ₇ H ₁₁ N	2-Methyl-5-vinylpyridine	1.467-100.93	342.77-456.34	8	4	Eng. Sci. Data Unit Boeblik, T., et al.	1973	B C	
30	C ₈ H ₁₁ N	N-Ethylaniline	0.001-3862.7	240.-675.	88	8	Eng. Sci. Data Unit	1978	C	
31	C ₈ H ₁₁ N	4-Ethylaniline	0.133-6.67 0.133-101.33	322.2-392.4 323.2-477.2	50 10	16 41	Eng. Sci. Data Unit Timmermans, J.	1965 1947	B C	
32	C ₈ H ₁₁ N	N,N-Dimethylaniline	0.133-101.33	270.-415. 323.2-479.3	90 32	41 66	Eng. Sci. Data Unit Nelson, O.A., et al.	1925 1973	A, Isoteniscopic C	
33	C ₈ H ₁₁ N	2-Ethylaniline	0.133-101.33	325.2-467.6	10	41	Eng. Sci. Data Unit Stull, D.R.	1947	C	
34	C ₈ H ₁₁ N	N,N-Dimethylaniline	0.010-3721.2	275.-685.	83	8	Eng. Sci. Data Unit	1965	C	
35	C ₈ H ₁₁ N	2,4-Dimethylaniline	0.009-3820.3	290.-710.	85	8	Eng. Sci. Data Unit	1978	C	
36	C ₈ H ₁₁ N	2,6-Dimethylaniline	0.009-3817.4	325.-848.7	88	8	Eng. Sci. Data Unit	1978	C	
37	C ₈ H ₁₁ N	2-Methyl-5-ethylpyridine	0.001-3272.6	325.-660.	86	8	Eng. Sci. Data Unit	1978	C	
38	C ₈ H ₁₁ N	2,4,6-Trimethylypyridine	0.001-3200.0	252.76-275.85	6	42	van De Rostyne, C., et al.	1960	A, Gas-saturation	10
39	C ₈ H ₁₁ N	2-Methyl-5-ethylpyridine	0.023-3232.8	260.-640.	77	8	Eng. Sci. Data Unit	1978	C	

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

No.	Formula	Name	Vapor Pressure Range, kPa ^a	Temperature Range, K	Number of Data Points	Reference	Authors	Year Published	Data Types & Methods of Measurement ^b	Reference Citing the Same Data Set ^c
38	C ₉ H ₇ N	Isoquinoline	13.412 ¹ 102.29 0.80 ² 101.33 0.003 ³ 4779.0	439.93 ⁴ 16.85 373.97 ⁵ 513.3 380.90 ⁶ 000.0 15.33 ⁷ 101.3 15.39 ⁸ 102.02	40 14 201 10 28	4 6 8 41 4	Boublik, T., et al. Coal Tar Res. Ass. Eng. Sci. Data Unit Stull, D.R. Boublik, T., et al. Coal Tar Res. Ass. Eng. Sci. Data Unit Timmermans, J. van De Rostyne, C., et al. Milne, J.W. M., et al.	1973 1965 1976 1947 1973 1965 1978 1965 1965 1981	B B C B B B B A, Gas-saturation A, Static	15 10 10
39	C ₉ H ₇ N	Quinoline	0.001 ¹ 3731.5 0.340 ² 101.3 0.340 ³ 99.37 0.0385 ⁴ 0.0243	348.5 ⁵ 510.7 348.5 ⁶ 780. 348.5 ⁷ 509.80 164.1 ⁸ 286.2 285.7 ⁹ 309.05	204 69 62 8 10	8 6 41 73 41	Eng. Sci. Data Unit Timmermans, J. van De Rostyne, C., et al. Milne, J.W. M., et al. Stull, D.R. Stull, D.R.	1978 1965 1976 1947 1947	C C C C C	10 10
40	C ₉ H ₁₃ N	4-Cumidine	0.133 ¹ 101.3	332.9 ² 510.9 333.1 ³ 500.15	10	41	Stull, D.R.	1947	C	10
41	C ₉ H ₁₃ N	4-Isopropylaniline	0.003 ¹ 3238.6	280. ² 715.	68	8	Eng. Sci. Data Unit	1978	C	
42	C ₉ H ₁₃ N	N,N ₂ -Triethylaniline	0.001 ¹ 3723.7 0.133 ² 101.3 0.133 ³ 101.3	245. ⁴ 765. 202. ⁵ 458.0 202. ⁶ 458.0	65 47 10	8 16 41	Eng. Sci. Data Unit Timmermans, J. Stull, D.R.	1978 1965 1947	C C C	
43	C ₉ H ₁₃ N	N,N ₄ -Trimethylaniline	0.001 ¹ 3750.0 0.133 ² 101.3 0.133 ³ 101.3	265. ⁷ 725. 323. ⁸ 482.7 323. ⁹ 482.7	87 10 10	8 41 41	Eng. Sci. Data Unit Stull, D.R. Eng. Sci. Data Unit	1978 1947 1978	C C C	
44	C ₉ H ₁₃ N	2,4,5-Trimethylaniline	0.154 ¹ 3500.0 0.133 ² 101.33 0.133 ³ 101.33	340. ⁶ 725. 345. ⁷ 507.7 345. ⁸ 507.7	78 10 25	8 41 41	Eng. Sci. Data Unit Stull, D.R. Eng. Sci. Data Unit	1978 1947 1978	C C C	15 15
45	C ₁₀ H ₉ N	3-Methylisoquinoline	0.001 ¹ 4956.9	285. ² 727.74	205	8	Eng. Sci. Data Unit	1978	C	
46	C ₁₀ H ₉ N	2-Methylquinoline	0.001 ¹ 4800.8 0.133 ² 101.33 0.133 ³ 101.33	280. ³ 785. 348.45 ⁴ 519.65 348.45 ⁵ 19.65	202 10 201	8 41 41	Eng. Sci. Data Unit Stull, D.R. Eng. Sci. Data Unit	1978 1947 1978	C C C	10, 15
47	C ₁₀ H ₉ N	4-Methylquinoline	0.001 ¹ 4554.4	295. ⁷ 795.	201	8	Eng. Sci. Data Unit	1978	C	
48	C ₁₀ H ₉ N	6-Methylquinoline	16.719 ¹ 101.75 0.001 ² 1684.2	471.73 ³ 38.97 265. ⁴ 745. 265. ⁵ 643.39.29	22 25 202	4 4 4	Boublik, T., et al. Boublik, T., et al. Eng. Sci. Data Unit	1973 1973 1978	S S C	15 15
49	C ₁₀ H ₉ N	7-Methylquinoline	0.001 ¹ 3658.2	290. ⁶ 925.	202	8	Eng. Sci. Data Unit	1978	C	
50	C ₁₀ H ₉ N	8-Methylquinoline	63.168 ¹ 101.90 61.723 ² 101.87	511. ⁷ 531.15 290. ⁷ 790.	17 201	4 4	Boublik, T., et al. Boublik, T., et al.	1973 1973	S S	15 15
51	C ₁₀ H ₉ N	1-Naphthylamine	0.001 ¹ 4950.8	500. ⁴ 48 ⁵ 21.30	16	4	Eng. Sci. Data Unit	1973	C	
52	C ₁₀ H ₉ N	2-Naphthylamine	0.005 ¹ 385.56	280. ⁷ 90. 325. ⁷ 645.	203 65	8 8	Eng. Sci. Data Unit Eng. Sci. Data Unit	1978 1978	C C	
53	C ₁₀ H ₉ N	Quinaldine	15.325 ¹ 101.62 0.00143 ² 0.0180	451.45 ³ 21.01 281.90 ⁴ 312.64	41 9	4 42	Boublik, T., et al. van De Rostyne, C., et al.	1973 1980	B A, Gas-saturation	
54	C ₁₀ H ₁₂ N	N,N-Diethylaniline	0.001 ¹ 1684.2 0.133 ² 101.33 0.133 ³ 101.33	265. ⁷ 645. 213. ⁸ 568.7 213. ⁹ 568.7	77 30 30	4 41 41	Eng. Sci. Data Unit Stull, D.R. Nelson, G.A., et al.	1978 1973 1925	C C A, Imbibitional	15
55	C ₁₁ H ₁₁ N	2,4-Dimethylquinoline	11.79 ¹ 106.53 0.001 ¹ 3826.2	458. ⁵ 542.60 295. ⁶ 805.	19 203	4 8	Boublik, T., et al. Eng. Sci. Data Unit	1973 1978	S C	15
56	C ₁₁ H ₁₁ N	2,6-Dimethylquinoline	13.416 ¹ 100.66 0.001 ² 3753.3	461.61 ³ 59.44 290. ⁷ 800.	27 203	4 6	Boublik, T., et al. Eng. Sci. Data Unit	1973 1978	S C	15
57	C ₁₂ H ₉ N	Carbazol	0.133 ¹ 101.62 7.37 ² 89.19	525. ⁷ 630.96 518. ⁷ 635.2	32 14	4 4	Boublik, T., et al. Coal Tar Res. Ass.	1973 1965	S B	10, 15
58	C ₁₂ H ₁₁ N	Diphenylamine	0.003 ¹ 555.48 60.00 ² 72.26	330. ⁷ 670. 551. ⁷ 558.	69 8	8 16	Eng. Sci. Data Unit Timmermans, J.	1978 1965	C B	
59	C ₁₃ H ₉ N	Acridine	0.133 ¹ 101.33 0.650 ² 0.1.070 ³	301.45 ³ 575.15 281.11 ⁷ 323.15	10 11	41 29	Stull, D.R. McEachern, D.M., et al.	1947 1975	C A	10
60	C ₁₃ H ₁₁ N	N-methyl diphenylamine	0.133 ¹ 101.33 0.133 ² 101.33	402.67 ³ 619.3 376. ⁷ 555.2	10 10	41 41	Stull, D.R. Stull, D.R.	1947 1947	C C	6, 10, 15
61	C ₁₄ H ₁₃ N	N-Ethylcarbazol	0.00247 ¹ 0.0147	347.81 ² 373.80	7	42	van De Rostyne, C., et al.	1980	A, Gas-saturation	
62	C ₁₄ H ₁₃ N	N-Ethyl diphenylamine	0.001 ¹ 583.05	310. ⁷ 670.	73	8	Eng. Sci. Data Unit	1978	C	
63	C ₁₄ H ₁₅ N	Dibenzylamine	0.001 ¹ 492.57 0.133 ² 101.33	320. ⁷ 670. 391.5 ⁷ 573.2.	71 10	8 41	Eng. Sci. Data Unit Stull, D.R.	1978 1947	C C	
64	C ₁₄ H ₁₇ N	N-methyl diphenylaniline	0.001 ¹ 623.62	310. ⁷ 670.	73	8	Eng. Sci. Data Unit	1978	C	

^a 1 kPa = 7.50062 torr (mm Hg).^b b

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.

^c Buill. = Builliometric

Table 7. Vapor pressure data on nitrogen compounds-II

No.	Formula	Name	Vapor Pressure Range, kPa ^a	Temperature Range, K	Number of Data Points	Reference	Authors	Year Published	Data Types ^b , Methods of Measurement
1	C ₄ H ₄ N ₂	Pyrazine	12.755~5673.0	330.~620.	59	8	Eng. Sci. Data Unit	1978	C
2	C ₄ H ₁₀ N ₂	Piperazine	0.165~4553.3	270.~655.	61	8	Eng. Sci. Data Unit	1978	C
3	C ₅ H ₆ N ₂	2-Methylpyrazine	2.392~4777.6	310.~630.	65	8	Eng. Sci. Data Unit	1978	C
4	C ₅ H ₁₂ N ₂	1-Methylpiperazine	0.001~4550.0	230.~630.	81	8	Eng. Sci. Data Unit	1978	C
5	C ₆ H ₈ N ₂	1,3-Diaminobenzene	0.012~1587.7	340.~720	77	8	Eng. Sci. Data Unit	1978	C
6	C ₆ H ₈ N ₂	1,3-Phenylenediamine	0.133~101.33	373.0~558.7	10	41	Stull, D.R.	1947	C
7	C ₆ H ₈ N ₂	Phenylhydrazine	0.133~101.33	345.~491.4	10	41	Stull, D.R.	1947	C
8	C ₆ H ₁₄ N ₂	cis-2,5-Dimethylpiperazine	..137~12.00 0.103~3000.0	373.~465. 290.~635.	70	69 8	Williams, G.E., et al. Eng. Sci. Data Unit	1942 1978	A&C, Isoteniscopic C
9	C ₇ H ₁₀ N ₂	4-Amino-2,6-dimethylpyridine	20.251~3820.7	460.~745.	58	8	Eng. Sci. Data Unit	1978	C
10	C ₇ H ₁₀ N ₂	2,4-Diaminotoluene	0.091~1440.6	375.~720.	70	8	Eng. Sci. Data Unit	1978	C
11	C ₈ H ₁₈ N ₂	Tetramethylpiperazine	0.001~2488.2 0.133~101.33	295.~645. 296.9~456.7	71 10	8 41	Eng. Sci. Data Unit Stull, D.R.	1978 1947	C C
12	C ₁₀ H ₁₄ N ₂	1-Phenylpiperazine	0.001~561.33	300.~655.	72	8	Eng. Sci. Data Unit	1978	C
13	C ₁₂ H ₈ N ₂	Phenazine	0.48x10 ⁻⁶ .23x10 ⁻⁵	281.11~323.15	12	29	McEachern, D.M., et al.	1975	A (solid)
14	C ₁₂ H ₁₀ N ₂	Azobenzene	0.133~101.33	376.7~566.2	10	41	Stull, D.R.	1947	C
15	C ₁₃ H ₁₄ N ₂	Di-(4-aminophenyl)-methane	0.001~325.17	375.~720.	70	8	Eng. Sci. Data Unit	1978	C
16	C ₃ H ₃ NO	Isoxazole	0.001~3741.8	195.~550.	72	8	Eng. Sci. Data Unit	1978	C
17	C ₃ H ₃ NO	Oxazole	0.001~3629.1	180.~510.	67	8	Eng. Sci. Data Unit	1978	C
18	C ₆ H ₅ NO ₃	2-Nitrophenol	0.133~101.33	322.5~487.7	10	41	Stull, D.R.	1947	C

^a 1 kPa = 7.50062 torr (mm Hg)^b

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 ^a	Temperature Range, K	Number of Data Points	Reference Number	Author(s)	Year Published	Data Types and Method of Measurement ^b	Reference Citing the Same Data ^c
1	C ₄ H ₈ O	Furan	31.16 ² 70.11 0.082 ⁵ 50.00	275.70 ² 334.580 193.15 ⁴ 480.25	13	4	Boublik, T., et al.	1973	B	
2	C ₆ H ₁₀ O	Cyclobutanone	62.00 ² 122.5	249.07 ² 296.29	22	14	Kudchadker, A.P., et al.	1978	B	
3	C ₆ H ₁₀ O	Tetrahydrofuran	0.267 ⁵ .760	295.00 ² 372.850	1	51	Kobe, K.A., et al.	1956	A, Static	15
4	C ₆ H ₁₀ O	2-Methylfuran	1.95 ⁴ 190.0	253.15 ² 372.850	15	4	Boublik, T., et al.	1973	B	
5	C ₆ H ₁₀ O	Cyclopentanone	35.00 ² 100.0	385.00 ² 527.62	27	51	Kobe, K.A., et al.	1956	A, Static	15
6	C ₆ H ₁₀ O	2-Methyl-tetrahydrofuran	0.307 ¹ 1.600	427.61 ² 533.17	4	4	Boublik, T., et al.	1973	B	
7	C ₆ H ₁₀ O	Phenoxy	634.33 ² 557.75	345.72 ² 481.57	20	51	Kobe, K.A., et al.	1956	A, Static	15
			1.33 ¹ 199.98	380.72 ² 481.57						
			7.605 ¹ 101.33	345.72 ² 481.57						
			0.00373 ¹ 0.27	273.15 ² 455.33	33	4	Boublik, T., et al.	1973	B	
			0.00384 ¹ 0.26	252.25 ² 659.25	20	6	Coal Tar Res. Ass.	1965	S	15
			0.00384 ¹ 0.26	252.25 ² 659.25	20	11	Kudchadker, A.P., et al.	1977	C	
			0.93 ³ 93751	252.25 ² 659.25	79	18	Timmermans, J.	1965	C	
8	C ₆ H ₁₂ O	Cyclohexanone	0.13 ³ 6.070	340.95 ² 691.15	19	1	Stull, D.R.	1947	C	
9	C ₆ H ₁₂ O	Cyclohexanol	12.725 ¹ 31.422	362.78 ² 748.92	16	31	Meyer, E.F., et al.	1947	A, Ebulliometric	10
10	C ₆ H ₁₂ O	2-Hexanone	0.13 ³ 1.01.33	394.15 ² 743.15	10	41	Stull, D.R.	1947	C	
			7.605 ¹ 101.33	394.15 ² 743.15	15	41	Shuzzo, O.	1947	C	
			0.13 ³ 1.01.33	394.15 ² 743.15	15	15	Boublik, T., et al.	1973	B	
			7.605 ¹ 101.33	394.15 ² 743.15	15	15	Timmermans, J.	1965	C	
			9.4 ⁴ 9.7.32	446.92 ² 324.92	7	1	Stull, D.R.	1947	C	
			0.13 ³ 1.01.33	395.15 ² 743.15	10	41	Timmermans, J.	1965	C	
12	C ₆ H ₁₀ O	Methoxybenzene (Anisole)	6.287 ⁶ 7.661	346.49 ² 412.52	6	16	Stull, D.R.	1947	C	15, 17
13	C ₆ H ₁₀ O	Benzylalcohol	0.287 ⁶ 7.661	334.05 ² 463.65	19	16	Timmermans, J.	1965	B	15
14	C ₆ H ₁₀ O	2-Hydroxytoluene (2-Cresol)	1.33 ³ 1.01.33	386.12 ² 575.65	10	41	Timmermans, J.	1965	B	
			10.11 ¹ 1.01.33	393.37 ² 654.10	5	4	TCHP	1978	C	
			0.00267 ¹ 0.04.98	271.15 ² 655.51	26	6	Stull, D.R.	1973	B	
			0.007479 ¹ 0.04.98	281.25 ² 697.65	28	6	Coal Tar Res. Ass.	1965	S	
			0.13 ³ 6.667	309.75 ² 838.45	49	16	Kudchadker, A.P., et al.	1978	C	
			0.13 ³ 1.01.33	311.35 ² 843.95	10	41	Timmermans, J.	1965	C	
			1.33 ³ 1.01.33	360.90 ² 933.65	27	2	TCHP	1978	C	
			20.22 ¹ 22.93	310.25 ² 822.25	22	4	Stull, D.R.	1947	C	
			0.00213 ¹ 0.05.53	273.15 ² 76.93	26	4	Coal Tar Res. Ass.	1965	S	10, 15
			0.00479 ¹ 0.05.53	283.25 ² 705.85	29	1	Kudchadker, A.P., et al.	1978	C	
			4.119 ¹ 124.29	386.12 ² 935.63	15	32	Nasir, P., et al.	1947	A, Static	
			0.13 ³ 1.01.33	386.12 ² 935.63	10	41	Stull, D.R.	1947	C	
			0.00235 ¹ 0.04.98	271.15 ² 655.51	26	6	Coal Tar Res. Ass.	1965	S	
			0.13 ³ 6.667	309.75 ² 838.45	49	16	Timmermans, J.	1965	C	
			0.13 ³ 1.01.33	311.35 ² 843.95	10	41	Stull, D.R.	1947	C	
			1.33 ³ 1.01.33	360.90 ² 933.65	27	2	TCHP	1978	C	
			20.22 ¹ 22.93	310.25 ² 822.25	22	4	Stull, D.R.	1947	C	
15	C ₆ H ₁₀ O	3-Hydroxytoluene	0.00213 ¹ 0.05.53	273.15 ² 76.93	10	41	Coal Tar Res. Ass.	1965	S	10, 15
			0.00479 ¹ 0.05.53	283.25 ² 705.85	29	1	Kudchadker, A.P., et al.	1978	C	
			4.119 ¹ 124.29	386.12 ² 935.63	15	32	Nasir, P., et al.	1947	A, Static	
			0.13 ³ 1.01.33	386.12 ² 935.63	10	41	Stull, D.R.	1947	C	
			0.00235 ¹ 0.04.98	271.15 ² 655.51	26	6	Coal Tar Res. Ass.	1965	S	
			0.13 ³ 6.667	309.75 ² 838.45	49	16	Timmermans, J.	1965	C	
			0.13 ³ 1.01.33	311.35 ² 843.95	10	41	Stull, D.R.	1947	C	
			1.33 ³ 1.01.33	360.90 ² 933.65	27	2	TCHP	1978	C	
			20.22 ¹ 22.93	310.25 ² 822.25	22	4	Stull, D.R.	1947	C	
17	C ₆ H ₁₀ O	Coumarone	0.01077 ⁰ 1.60.40	273.15 ² 313.15	7	41	Coal Tar Res. Ass.	1965	S	10
18	C ₆ H ₁₀ O	Acetophenone	1.373 ³ 2.53	352.65 ² 370.85	39	16	Timmermans, J.	1965	C	
19	C ₆ H ₁₀ O	2-Ethylphenol	0.13 ³ 1.01.33	310.25 ² 75.65	19	1	Stull, D.R.	1947	C	10
20	C ₆ H ₁₀ O	3-Ethylphenol	0.13 ³ 1.01.33	319.35 ² 80.65	10	41	Stull, D.R.	1947	C	10
21	C ₆ H ₁₀ O	4-Ethylphenol	0.00098 ¹ 0.04.98	278.15 ² 491.19	28	15	Boublik, T., et al.	1973	B	6
22	C ₆ H ₁₀ O	2,3-Dimethylphenol	0.00335 ¹ 0.04.98	313.35 ² 490.65	10	41	Shuzzo, O.	1947	C	10
			1.33 ³ 1.01.33	313.35 ² 490.65	10	41	TCHP	1978	C	
			0.000322 ¹ 0.04.98	281.25 ² 704.65	29	12	Boublik, T., et al.	1973	C	
			0.13 ³ 6.667	328.85 ² 394.45	50	16	Timmermans, J.	1965	C	
			0.13 ³ 1.01.33	326.15 ² 474.95	10	41	Stull, D.R.	1947	C	
			0.01077 ⁰ 1.60.40	273.15 ² 313.15	7	41	Coal Tar Res. Ass.	1965	S	
			0.00213 ¹ 0.05.53	283.25 ² 705.85	29	1	Kudchadker, A.P., et al.	1978	C	
			4.119 ¹ 124.29	386.12 ² 935.63	15	32	Nasir, P., et al.	1947	A, Static	
			0.13 ³ 1.01.33	386.12 ² 935.63	10	41	Stull, D.R.	1947	C	
			0.00235 ¹ 0.04.98	271.15 ² 655.51	26	6	Coal Tar Res. Ass.	1965	S	
			0.13 ³ 6.667	309.75 ² 838.45	49	16	Timmermans, J.	1965	C	
			0.13 ³ 1.01.33	311.35 ² 843.95	10	41	Stull, D.R.	1947	C	
			1.33 ³ 1.01.33	360.90 ² 933.65	27	2	TCHP	1978	C	
			20.22 ¹ 22.93	310.25 ² 822.25	22	4	Stull, D.R.	1947	C	
23	C ₆ H ₁₀ O	2,4-Dimethylphenol	1.33 ³ 1.01.33	313.35 ² 487.15	10	41	Coal Tar Res. Ass.	1965	S	
			0.00098 ¹ 0.04.98	278.15 ² 704.62	28	13	Kudchadker, A.P., et al.	1978	C	
			0.13 ³ 6.667	328.05 ² 513.40	50	16	TCHP	1978	C	
			0.13 ³ 1.01.33	328.05 ² 513.40	50	16	Arden, R.J.L., et al.	1960	A, Ebulliometric	6, 15
			0.00061 ¹ 0.05.40	281.05 ² 521.62	52	2	TCHP	1978	C	
			0.00190 ¹ 0.04.98	278.27 ² 707.65	29	13	Kudchadker, A.P., et al.	1978	C	
			0.13 ³ 6.667	328.95 ² 524.65	50	16	Stull, D.R.	1947	C	
			0.13 ³ 1.01.33	328.95 ² 524.65	50	16	TCHP	1978	C	
			0.000304 ¹ 0.04.98	282.88 ² 485.47	30	13	Arden, R.J.L., et al.	1960	A, Ebulliometric	10
			24.34 ³ 50.28	324.95 ² 523.67	18	73	Wilson, G.M., et al.	1981	A, Static	
			1.33 ³ 1.01.33	325.60 ² 523.39	19	2	TCHP	1978	C	
			0.000336 ¹ 0.04.98	285.60 ² 523.39	27	12	Kudchadker, A.P., et al.	1978	C	
			0.13 ³ 1.01.33	329.95 ² 487.65	10	41	Stull, D.R.	1947	C	
			0.00060 ¹ 0.05.40	282.58 ² 484.89	50	58	Arden, R.J.L., et al.	1960	A, Ebulliometric	4, 6, 15
			1.33 ³ 1.01.33	353.85 ² 503.66	27	2	TCHP	1978	C	
			0.00267 ¹ 0.04.98	278.27 ² 704.62	28	13	Kudchadker, A.P., et al.	1978	C	
			0.13 ³ 6.667	328.75 ² 526.68	52	2	Arden, R.J.L., et al.	1960	A, Ebulliometric	4, 6, 15
			0.13 ³ 1.01.33	328.75 ² 526.68	52	2	TCHP	1978	C	
			0.000155 ¹ 0.05.00	282.88 ² 496.35	29	13	Kudchadker, A.P., et al.	1978	C	
			0.13 ³ 1.01.33	339.35 ² 496.35	10	41	Stull, D.R.	1947	C	
			0.000293 ¹ 0.04.98	283.04 ² 03.05	30	13	Arden, R.J.L., et al.	1960	A, Ebulliometric	4, 6, 15
			1.33 ³ 1.01.33	376.55 ² 523.67	27	13	TCHP	1978	C	
			0.000242 ¹ 0.04.98	278.27 ² 715.65	28	13	Kudchadker, A.P., et al.	1978	C	
			0.13 ³ 6.667	328.75 ² 526.68	52	2	Stull, D.R.	1947	C	
			0.00044 ¹ 0.05.74	282.55 ² 494.41	51	1	Stull, D.R.	1947	C	10
			0.13 ³ 1.01.33	328.95 ² 524.65	50	6	TCHP	1978	C	
			0.00061 ¹ 0.05.40	284.85 ² 521.62	52	17	Arden, R.J.L., et al.	1960	A, Ebulliometric	4, 6, 15
			0.13 ³ 1.01.33	330.55 ² 521.62	50	10	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.⁻²) in the temperature range from 10–220 °F.² 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.*^{33,35} and was fitted to a Chebyshev polynomial.⁸ However, it is not convenient to obtain dP/dT from the Chebyshev polynomial vapor pressure equation for calculating enthalpy of vaporization (ΔH_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 follows¹⁹:

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

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 ^a	Temperature Range, K	Number of Data Points	Reference Number	Author(s)	Year Published	Data Type and Method of Measurement ^b	Reference Citing the same Data
1	C ₆ H ₅ Q	Quinone(-Benzquinone)	0.280–2.027	259.85–278.45	4	16	Timmermans, J.	1965	B	
2	C ₆ H ₅ Q ₂	1,2-Dihydroxibenzene (Pyrocatechol)	1.333–101.33	391.65–518.65	19	4	Boulik, T., et al.	1973	B	
3	C ₆ H ₅ Q	1,3-Dihydroxybenzene (Resorcinol)	1.333–101.33	424.65–549.65	19	41	Boulik, D.R.	1947	C	
4	C ₆ H ₅ Q	1,4-Dihydroxybenzene (Hydroquinone)	0.133–101.33	381.55–549.65	10	4	Boulik, T., et al.	1973	B	
5	C ₆ H ₅ O	Pyrogallol	0.133–101.33	432.25–559.15	19	41	Boulik, D.R.	1947	C	
6	C ₇ H ₈ Q	Quinacrol	0.787–64.301	428.15–541.05	14	16	Timmermans, J.	1965	B	
7	C ₁₂ H ₈ O	DiPhenylene Oxide	0.133–101.33	405.55–575.35	10	41	Sull, D.R.	1947	B	
8	C ₁₂ H ₈ O	Dibenzofuran	0.133–101.33	450.45–592.15	19	4	Boulik, T., et al.	1973	B	
9	C ₁₂ H ₁₀ O ₂	2,2-Diphenol	0.133–101.33	424.85–592.15	10	41	Sull, D.R.	1947	C	
10	C ₁₂ H ₁₀ O ₂	Quinhydrone	0.133–101.33	355.15–578.15	19	4	Boulik, T., et al.	1973	B	
11	C ₁₄ H ₁₀ O ₂	Anthrathrone	0.622–171.714	398.35–558.25	19	6	Coal Tar Res. Ass.	1965	B	
			5.186–291.677	377.01–586.46	6	74	Nasir, P., et al.	1982	A, Static	
			1.333–101.33	435.35–618.05	19	75	Sivarajan, A., et al.	1982	A, Static	
			0.0043467–0.0020398	317.55–533.55	6	16	Boulik, T., et al.	1973	B	
			13.886–107.285	558.73–856.33	33	10	Timmermans, J.	1965	B	
							Jordan, T.E.	1954	C	

^a 1 kPa = 7.50062 torr (mm Hg).

^b 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	$\log_{10} P = (1 - D/T) \times 10 (A + BT + CT^2)^a$				Vapor Pressure Range, kPa	Temperature Range, K	Calculated Vapor Pressure kPa at 400.0 K	AAD ^b %	Number of Data	Data Reference Numbers
		A	B $\times 10^4$	C $\times 10^7$	D						
1	Benzene	0.832632	-6.72598	6.38324	353.214	5.13 ~ 4924.0	280.0~562.6	352.73	0.171	131	8, 17, 24, 35, 55
2	Toluene	0.837122	-6.48791	5.91293	383.737	0.119 ~ 4016.3	245.0~590.0	157.35	0.133	120	8, 52, 56, 60
3	Styrene	0.886470	-8.14267	7.57896	418.675	0.288 ~ 100.51	281.35~417.92	60.424	0.854	21	6
4	Ethylbenzene	0.859833	-6.85948	5.94439	409.229	0.0204 ~ 3507.0	243.2~615.0	78.549	0.424	127	8, 17, 56
5	2-Methyltoluene	0.855257	-6.48662	5.53883	417.496	0.0324 ~ 3808.0	253.2~631.64	62.263	0.347	127	8, 17, 56
6	3-Methyltoluene	0.858941	-6.73249	5.87438	412.135	0.0169 ~ 3650.0	243.2~619.2	72.326	0.513	156	6, 8, 17, 56
7	4-Methyltoluene	0.847730	-6.39489	5.59094	411.503	0.74 ~ 3617.0	290.0~618.2	73.728 ^c	0.103	112	8, 17, 56
8	2-Methylstyrene	0.890379	-7.17666	5.97058	443.504	0.387 ~ 17.70	305.16~385.5	28.979	0.145	9	4
9	3-Methylstyrene	0.885861	-7.19653	6.75359	442.985	0.687 ~ 99.725	314.93~442.15	28.811	0.774	27	4
10	4-Methylstyrene	0.875061	-7.08160	7.33467	443.748	0.133 ~ 99.725	289.15~443.15	27.919	0.733	31	4, 41
11	n-Propylbenzene	0.891023	-6.89092	5.79948	432.321	0.133 ~ 3078.1	280.0~635.0	40.890	0.128	91	4, 8
12	Isopropylbenzene	0.877964	-7.23971	6.06942	425.438	0.057 ~ 3166.0	264.95~630.0	49.827	0.382	127	6, 8, 16
13	1-Methyl-2-ethylbenzene	0.863837	-6.34917	5.19164	438.357	0.141 ~ 3206.6	285.0~645.0	34.109	0.077 ^c	93	4, 8
14	1-Methyl-3-ethylbenzene	0.861399	-6.30303	5.19848	434.538	0.118 ~ 3065.4	280.0~635.0	38.056	0.122	92	4, 8
15	1-Methyl-4-ethylbenzene	0.856105	-6.18307	5.08568	435.228	0.120 ~ 2977.6	280.0~635.0	37.516	0.159	91	4, 8
16	1,2,3-Trimethylbenzene	0.869047	-6.33423	5.14963	449.175	0.116 ~ 3283.3	290.0~660.0	24.677	0.178	75	8
17	1,2,4-Trimethylbenzene	0.846724	-5.41424	4.22211	442.537	0.00886~3076.9	253.0~645.0	30.109	0.866	108	6, 8, 10
18	1,3,5-Trimethylbenzene	0.872945	-6.55508	5.47586	437.769	0.00938~3046.47	253.0~635.0	34.219	0.964	117	6, 8, 10
19	n-Butylbenzene	0.889482	-7.01177	5.65027	456.368	0.1120 ~ 2870.90	295.0~660.0	19.971	0.557	102	4, 8, 41
20	Isobutylbenzene	0.870338	-6.75481	5.59009	445.940	0.105 ~ 2775.0	285.0~645.0	27.781	0.0507	93	4, 8
21	sec-Butylbenzene	0.870844	-6.72060	5.52698	446.499	0.101 ~ 2733.7	285.0~645.0	27.275	0.0691	93	4, 8
22	tert-Butylbenzene	0.881530	-7.21114	6.01764	442.319	0.119 ~ 2591.4	285.0~635.0	30.782	0.0656	90	4, 8
23	1-Methyl-2-propylbenzene	0.887506	-6.92975	5.60140	458.002	0.106 ~ 2827.0	295.0~660.0	19.014	0.0447	74	8
24	1-Methyl-3-propylbenzene	0.817457	-6.56228	5.30555	455.038	0.124 ~ 2670.8	295.0~650.0	25.427	0.131	99	2, 8
25	1-Methyl-4-propylbenzene	0.882883	-6.86216	5.57573	456.497	0.118 ~ 2705.5	295.0~655.0	20.032	0.0612	100	2, 8
26	1-Methyl-2-isopropylbenzene	0.877779	-6.88555	5.61774	451.343	0.112 ~ 2835.9	290.0~655.0	23.648	0.150	109	2, 4, 8
27	1-Methyl-3-isopropylbenzene	0.875856	-6.90589	5.71011	448.380	0.131 ~ 2652.8	290.0~645.0	25.822	0.274	107	2, 4, 8
28	1-Methyl-4-isopropylbenzene	0.875129	-6.86627	5.61507	450.311	0.121 ~ 2694.2	290.0~650.0	24.504	0.124	107	2, 4, 8
29	1,2-Diethylbenzene	0.885449	-6.81892	5.48568	456.641	0.112 ~ 2901.5	295.0~660.0	19.736	0.0892	94	4, 8
30	1,3-Diethylbenzene	0.889714	-6.94128	5.62739	454.362	0.119 ~ 2716.8	294.85~650.0	20.954	0.603	102	4, 8, 41
31	1,4-Diethylbenzene	0.893772	-7.13376	5.76066	456.809	0.107 ~ 2708.6	295.0~655.0	19.631	0.337	93	4, 8
32	1,2-Dimethyl-3-ethylbenzene	0.868962	-5.88268	4.49402	467.211	0.139 ~ 2956.5	305.0~675.0	11.215	0.234	102	2, 8
33	1,2-Dimethyl-4-ethylbenzene	0.888166	-6.72722	5.37774	462.948	0.114 ~ 2858.4	300.0~665.0	15.130	0.0639	101	2, 8
34	1,3-Dimethyl-2-ethylbenzene	0.891249	-6.82799	5.40578	463.219	0.112 ~ 2964.6	330.0~670.0	15.037	0.101	102	2, 8
35	1,3-Dimethyl-4-ethylbenzene	0.870425	-6.11874	4.78949	461.691	0.130 ~ 2852.5	300.0~665.0	15.938	0.227	101	2, 8
36	1,3-Dimethyl-5-ethylbenzene	0.892544	-7.07867	5.82215	456.921	0.117 ~ 2633.7	295.0~650.0	19.450	0.0751	99	2, 8
37	1,4-Dimethyl-2-ethylbenzene	0.867112	-6.40948	4.68254	460.129	0.101 ~ 3381.6	295.0~680.0	17.850	0.0997	105	2, 8
38	1,2,3,4-Tetramethylbenzene	0.889484	-6.47585	4.96841	478.255	0.111 ~ 2970.1	310.0~690.0	10.058	0.0988	104	2, 8
39	1,2,3,5-Tetramethylbenzene	0.891876	-6.64575	5.21861	471.208	0.106 ~ 2850.3	305.0~675.0	12.407	0.0721	102	2, 8
40	1,2,4,5-Tetramethylbenzene	0.884259	-6.36677	4.97446	470.032	1.333 ~ 2913.0	346.75~675.0	12.868	0.119	92	2, 8
41	sec-Amylbenzene	0.897853	-6.86006	7.72031	451.128	0.133 ~ 101.33	300.95~451.15	19.585	0.627	10	41
42	3-Ethyl-1-isopropylbenzene	0.859693	-6.82452	7.58198	465.962	0.133 ~ 101.33	301.45~446.15	14.582	0.370	10	41
43	4-Ethyl-1-isopropylbenzene	0.871494	-7.16782	8.01142	468.985	0.133 ~ 101.33	304.65~468.95	13.037	0.500	10	41
44	3,5-Diethyltoluene	0.865431	-7.13287	7.63657	472.018	0.133 ~ 101.33	304.95~472.15	12.355	0.617	10	41
45	1,2,4-Trimethyl-5-ethylbenzene	0.782663	-5.94151	18.3976	464.965	1.467 ~ 9.466	360.45~405.25	7.6514	2.75	11	4
46	1,3,5-Trimethyl-2-ethylbenzene	0.917293	-6.86816	4.53769	483.486	1.573 ~ 101.33	361.65~483.35	8.3653	1.05	19	4
47	1,2-Diisopropylbenzene	0.869528	-6.85396	7.42464	482.090	0.133 ~ 101.33	313.15~482.15	8.7959	0.437	10	41
48	1,3-Diisopropylbenzene	0.867688	-7.14442	8.11668	475.120	0.133 ~ 101.33	307.85~475.15	10.930	0.302	10	41
49	1,4-Diisopropylbenzene	0.900726	-6.87306	5.22622	483.33	6.753 ~ 104.63	393.41~484.73	8.6840	0.115	7	4
50	1,2,4-Triethylbenzene	0.881965	-7.59082	8.58854	491.389	0.133 ~ 101.33	319.15~491.15	6.5820	0.751	10	41
51	1,3,4-Triethylbenzene	0.879248	-6.92921	7.78309	490.542	0.133 ~ 101.33	321.05~490.65	6.3034	0.664	10	41
52	Hexamethylbenzene	1.00973	-5.04725	-6.30130	571.163	0.00028~0.0144	303.10~343.02	0.6701	0.533	9	48

^a P in atm (1.01325 bar or 101.32 kPa); K in T.

^b AAD = absolute average deviation = $\frac{\sum | \text{Calculated value} - \text{Experimental value} |}{\text{number of data points}}$

^c 400 K outside the temperature range of the data used in evaluating the coefficient of the vapor pressure equation.

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

No.	Name	$\log_{10} P = (1 - D/T) \times 10^4 (A + BT + CT^2)^a$				Vapor Pressure Range, kPa	Temperature Range, K	Calculated Vapor Pressure kPa at 400.0 K	AAD ^b %	Number of Data Points	Data Reference Number
		A	B $\times 10^4$	C $\times 10^7$	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	0.00176~415.36	278.85~593.38	3.0627	0.366	93	2, 6, 53
3	2-Methylnaphthalene	0.879050	-5.85793	4.19253	514.242	1.33300~735.96	378.00~529.32	3.4264	0.195	89	2, 4, 6, 53
4	1-Ethylnaphthalene	0.923623	-6.97505	5.07450	531.480	1.33300~199.98	393.15~565.45	1.8090	0.0358	27	2
5	2-Ethylnaphthalene	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 ^c	0.113	23	2
7	1,3-Dimethylnaphthalene	1.72680	-7.87991	-42.8535	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	328.15~413.15	1.0306	1.89	20	38
10	2,3-Dimethylnaphthalene	1.09999	-10.2378	-11.3931	631.969	0.01400~1.8534	333.15~408.15	1.3707	3.92	16	38
11	2,6-Dimethylnaphthalene	1.14901	-11.9220	-17.3468	687.081	0.05367~3.4419	328.15~418.15	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 ^c	5.87	15	38
13	1-n-Propylnaphthalene	1.01439	-7.21205	0.0344076	546.126	1.33300~101.33	403.15~545.95	1.1476 ^c	0.525	10	2
14	2-n-Propylnaphthalene	1.02538	-7.12594	-0.699309	546.808	1.33300~101.33	404.15~546.65	1.0928 ^c	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 ^c	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 ^c	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 ^c	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 ^c	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 ^c	1.20	7	2
20	1-n-Butylnaphthalene	1.10895	-7.77663	-4.60035	563.025	1.33300~106.66	412.85~565.95	0.70084 ^c	1.28	23	2
21	2-n-Butylnaphthalene	0.971423	-6.86834	3.12397	561.352	1.33300~106.66	418.15~564.15	0.56340 ^c	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 ^c	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 ^c	0.665	23	2

^a P in atm (1.01325 bar or 101.325 kPa); T in K.

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

^c 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	$\log_{10} P = (1 - D/T) \times 10^3 + (A+B+CT^2)^a$				Vapor Pressure Range, kPa	Temperature Range, K	AAD ^b %	Number of Data Points	Reference Number	Pressure kPa at 400 K
		A	B $\times 10^4$	C $\times 10^7$	D						
1	Cyclopropane	0.764677	-6.98761	9.83198	240.301	1.333-5579.5	171.85-398.3	0.188	65	2, 4, 54	5734.5 ^c
2	Cyclobutane	0.887736	-15.1134	24.6051	285.734	0.133-199.98	181.15-305.66	0.770	62	2, 4, 41, 70	2307.9 ^c
3	Methylcyclobutane	0.861895	-10.8963	10.8762	278.061	0.133-101.33	177.15-277.65	0.021	10	41	1657.7 ^c
4	Cyclopentane	0.818603	-7.52365	8.27395	322.386	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	353.663	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	-9.88091	10.8367	344.830	0.0019-2924.0	183.15-53.15	0.848	60	2, 17	419.03
7	Cycloheptane	0.865524	-8.19621	7.88065	391.896	1.33-270.11	284.35-432.17	0.396	42	2, 4	125.64
8	Ethylcyclopentane	0.839111	-7.11414	6.79653	376.588	1.333-3143.0	273.24-563.15	0.151	77	2, 4, 17	188.49
9	1,1-Dimethylcyclopentane	0.883976	-10.8001	12.4624	361.619	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	372.619	4.00-199.98	291.15-398.35	1.631	45	2, 4	205.69
11	1,trans-2-Dimethylcyclopentane	0.849992	-8.27119	8.67505	365.020	1.333-199.98	264.15-390.25	0.044	45	2, 4	253.25 ^c
12	1,cis-3-Dimethylcyclopentane	0.835365	-8.23938	10.1173	364.284	1.333-199.98	263.15-389.15	1.40	45	2, 4	263.71 ^c
13	1,trans-3-Dimethylcyclopentane	0.863033	-8.40761	7.45113	364.572	1.333-199.98	263.15-390.15	1.399	46	2, 4	249.84 ^c
14	Methylcyclohexane	0.862568	-8.71426	8.69685	373.957	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	404.971	0.033-310.80	243.20-453.20	0.394	57	2, 17, 41	88.698
16	1,1-Dimethylcyclohexane	0.803626	-5.20532	3.85619	392.673	0.133-199.98	248.75-420.25	0.346	57	2, 4, 41	122.71
17	1,cis-2-Dimethylcyclohexane	0.841813	-6.56119	5.01855	402.894	0.133-199.98	257.25-430.75	0.476	57	2, 4, 41	93.902
18	1,trans-2-Dimethylcyclohexane	0.827486	-6.12608	4.53086	396.346	0.133-199.98	252.05-424.25	1.11	37	2, 41	111.43
19	1,cis-3-Dimethylcyclohexane	0.841956	-7.14598	6.48250	393.241	0.133-199.98	250.45-420.55	0.137	37	2, 41	121.04
20	1,trans-3-Dimethylcyclohexane	0.840923	-6.82912	5.97404	397.599	0.133-199.98	253.75-425.05	0.149	37	2, 41	107.99
21	1,cis-4-Dimethylcyclohexane	0.8266432	-6.13308	5.14765	397.443	0.133-199.98	253.15-424.95	0.230	37	2, 41	108.44
22	1,trans-4-Dimethylcyclohexane	0.826623	-6.77160	6.50408	392.510	0.133-199.98	248.85-4.9.95	0.187	37	2, 41	123.39
23	Isopropylcyclopentane	0.861708	-8.18102	8.29785	399.575	1.333-199.98	289.55-426.95	0.032	47	2, 4	102.48
24	Propylcyclopentane	0.856232	-7.04448	6.25094	404.097	1.333-199.98	294.45-431.35	0.051	46	2, 4	90.639
25	1-Ethyl-1-methylcyclopentane	0.835292	-6.58763	5.67554	394.712	0.042-270.02	238.15-435.30	0.391	52	4, 34	116.55
26	cis-2-Ethyl-1-methylcyclopentane	0.855851	-7.83360	11.3549	394.617	0.028-1.114	238.15-288.15	0.234	11	34	119.41 ^c
27	1,1,2-Trimethylcyclopentane	0.853137	-8.19842	8.40843	386.878	1.333-199.98	279.53-4.3.75	0.026	46	2, 4	143.08
28	1,1,3-Trimethylcyclopentane	0.848231	-8.28174	8.81168	378.065	1.333-199.98	272.85-404.45	0.184	46	2, 4	179.97
29	Propylcyclohexane	0.865420	-7.04026	5.98962	429.890	1.333-199.98	313.35-458.95	0.050	47	2, 4	44.499
30	Isopropylcyclohexane	0.876667	-7.99142	7.47343	427.713	6.411-104.01	343.66-428.75	0.013	20	4	47.502
31	cis-3-Ethyl-1-methylcyclohexane	0.843964	-6.42051	5.49912	421.619	9.59-269.98	348.31-464.42	0.011	21	34	56.223
32	1,1,2-Trimethylcyclohexane	0.838270	-6.63916	5.61172	409.802	6.40-104.00	327.82-4.0.80	0.286	25	4, 50	78.174
33	n-Butylcyclohexane	0.891776	-7.48841	6.21822	454.131	1.333-199.98	332.65-484.35	0.061	27	2	21.891
34	Isobutylcyclohexane	0.848267	-6.44098	5.35931	427.717	6.41-104.01	343.66-428.75	0.021	20	4	47.514
35	sec-Butylcyclohexane	0.925582	-7.13653	2.83949	452.650	6.41-104.01	376.61-453.57	1.37	20	4	23.314
36	tert-Butylcyclohexane	0.882098	-7.99990	7.31667	444.737	6.40-104.00	357.18-415.82	0.022	20	4	29.609

^a P in Atm(1.01325 bar or 101.325 kPa); T in K

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

^c 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 pressure at 400 K for unsaturated ring compounds

No.	Name	$\log_{10} P = (1 - D/T) \times 10^{(A+B+CT^2)^a}$				Vapor Pressure Range, kPa	Temperature Range, K	AAD ^b %	Number of Data Points	Reference Number	Pressure kPa, at 400 K
		A	B $\times 10^4$	C $\times 10^7$	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 ^c
2	1,3-Cyclopentadiene	0.919018	-8.68344	-3.41259	314.762	18.82-96.33	271.25-313.05	0.055	20	15	508.88 ^c
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 ^c
4	1,3-Cyclohexdiene	0.823433	-6.73214	6.67096	353.486	16.80-135.20	303.96-343.31	0.152	19	27, 31	345.40 ^c
5	1,4,-Cyclohexdiene	0.916704	-6.81678	-7.02362	368.566	11.89-25.25	304.25-322.23	0.206	7	27	187.51 ^c
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 ^c
7	Indene	0.796974	-5.99769	9.52748	155.041	0.133-104.41	289.55-456.97	1.46	20	6, 41	19.990
8	Indan	0.859420	-6.08324	4.77502	451.051	4.34-104.41	355.01-452.24	0.169	50	6, 26, 37	23.825
9	Tetralin	0.859186	-5.75417	4.41972	480.364	0.133-3364.64	311.15-710.93	1.589	46	4, 16, 32, 41, 73	9.9861
10	cis-Decalin	0.683577	0.900942	-2.28255	468.915	0.133-3571.48	295.65-727.59	2.136	46	4, 41, 73	14.969
11	trans-Decalin	0.860979	-6.38749	4.59180	460.458	5.53-102.73	365.51-461.02	0.463	19	4	19.233
12	1,1-Dimethylindan	0.869995	-6.14831	4.52781	467.243	0.258-101.33	313.15-467.22	0.037	24	37	14.789
13	4,6-Dimethylindan	0.887063	-6.04521	4.35551	498.089	0.057-47.38	313.15-467.22	0.144	18	37	5.4159
14	4,7-Dimethylindan	0.887652	-6.04765	4.32653	501.078	0.050-47.38	313.15-469.96	0.160	17	37	4.9525
15	Biophenylene	1.11763	-8.19240	-13.7006	601.351	0.027-1.835	343.15-408.15	4.28	15	56	1.3564
16	Byphenyl	0.821470	-2.73337	1.02285	528.437	0.104-1108.57	342.35-673.15	1.298	85	4, 6, 72	1.9388
17	Phenylcyclohexane	0.914718	-8.43553	6.82927	508.790	264.8-2457.3	560.93-727.59	0.917	7	73	4.8321 ^c
18	Bicyclohexyl	0.876522	-5.41554	3.04865	510.926	0.066-346.09	321.20-517.25	0.959	28	1, 44	3.8708
19	1,1-Dicyclohexylethane	1.31737	-14.8631	14.2837	521.581	0.067-1.333	385.65-430.65	7.888	5	1	0.19413
20	Bi phenylmethane	0.918987	-6.39483	4.39313	537.844	0.066-1827.10	343.15-727.59	1.613	50	1, 16, 44, 73	1.3809
21	1,1,4,6-Tetramethylindan	0.908228	-6.35384	4.10220	508.143	0.032-38.565	313.15-468.80	0.482	18	37	3.8709
22	1,1,4,7-Tetramethylindan	0.895344	-6.09096	4.01316	517.025	0.025-31.177	313.15-468.80	0.186	18	37	3.0528
23	Bipheylethylene	1.09345	-16.2565	20.9352	534.786	0.067-1.333	350.15-407.15	0.384	5	1	0.96348
24	1,1-Diphenylethane	0.893301	-5.45280	8.02493	524.104	0.067-1.333	348.65-404.65	0.524	5	1	1.0761
25	1,2-Diphenylethane	0.914704	-6.08831	5.11258	547.288	0.017-1.498	333.15-413.15	0.403	17	56	0.83338
26	2-Butyltetralin	0.903037	-5.60471	9.29569	524.981	0.067-1.333	354.65-410.65	0.219	5	1	0.80356
27	1-Cyclohexyl-1-phenylethane	1.08057	-15.5344	24.1341	507.179	0.067-1.333	345.15-399.65	0.833	5	1	1.3460 ^c
28	2-Cyclohexyl-1-phenylethane	1.06923	-16.0395	22.9852	528.286	0.067-1.333	348.15-406.15	0.667	5	1	1.0079
29	3-Cyclopentyl-1-phenylpropane	1.07498	-16.0536	22.6935	528.173	0.067-1.333	348.65-406.15	0.701	5	1	1.0064
30	1,1-Dicyclopentylmethane	1.07652	-15.8050	23.4302	516.862	0.067-1.333	346.15-402.15	0.594	5	1	1.1995
31	1,2-Dicyclohexylmethane	1.07728	-15.4160	24.9170	506.850	0.067-1.333	347.75-402.15	0.972	5	1	1.1848

^a P in Atm(1.01325 bar or 101.325 kPa); T in K

^b AAD = absolute average deviation = $\Sigma | \text{Calculated value} - \text{experimental value} | / \text{experimental value}$ number of data points

^c 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	$\log P = (1 - D/T) \times 10^{(A+BT+CT^2)^a}$				Vapor Pressure Range, kPa	Temperature Range, K	AAD ^b %	Number of Data Points	Reference Number	Pressure kPa at 400 K
		A	B $\times 10^4$	C $\times 10^7$	D						
1	Thiacyclopropane	0.823181	-7.01267	7.70188	328.076	1.333-270.11	238.55-360.88	0.051	40	2, 4	690.01 ^c
2	Thiacyclobutane	0.880604	-9.52708	10.9166	368.152	1.333-270.11	268.25-401.79	0.090	57	2, 4, 36	240.84
3	Thiophene	0.901276	-10.3229	11.9393	394.395	1.333-270.11	287.35-433.60	0.436	61	2, 36, 43	118.22
4	Tetrahydrothiophene	0.851037	-7.11948	6.89859	394.281	1.333-199.98	287.35-420.61	0.134	32	2, 24	118.47
5	Thiacyclopentane	0.865149	-7.93338	7.59224	357.255	0.107-5467.5	228.15-577.61	1.354	145	2, 4, 6, 16, 41, 51	319.69
6	2-Methylthiophene	0.913733	-10.3914	11.2735	385.680	1.333-199.98	282.15-411.15	0.250	35	2, 24	150.13
7	3-Methylthiophene	0.803952	-5.13436	5.45565	388.532	0.133-199.98	248.65-414.15	1.385	45	2, 24, 41	139.58
8	Cyclopentanethiol	0.925892	-10.4911	10.6639	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	Benzene-thiol	0.928694	-9.23421	8.59363	442.321	1.333-270.11	235.43-485.11	0.075	57	2, 4, 36	30.152
13	2,5-Dimethylthiophene	0.885251	-10.3540	14.9835	407.929	7.40-34.26	333.45-371.45	0.047	5	24	80.141 ^c
14	2-Ethylthiophene	0.868809	-10.2879	16.6827	404.508	8.12-37.33	333.45-371.45	0.038	5	24	88.307 ^c
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	345.15-498.15	0.203	27	2	14.402
23	4-Methylbenzenethiol	0.922351	-8.74250	7.84906	468.114	1.333-199.98	343.15-499.15	0.315	27	2	14.313
24	1-Thiaethylbenzene	0.884670	-6.02526	4.25882	467.456	9.582-70.11	390.29-452.97	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	0.60153
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 ^c
27	Dibenzothiophene	0.865373	-5.51221	6.05701	605.160	0.471-105.90	424.81-607.53	0.405	19	75	0.14977 ^c

^a p in Atm (1.01325 bar or 101.325 kPa); T in K

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

^c 400 K is outside the temperature range of the data used in evaluating the coefficients of the vapor pressure equation.

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TABLE 15. Coefficients of vapor pressure equation and the calculated vapor pressures at 400 K for nitrogen compounds - I

No.	Name	$\log_{10} P = (1-D/T) \times 10^A + BT + CT^2$ ^a				Vapor Pressure Range, kPa	Temperature Range, K	Vapor Pressure kPa	AAD ^b %	Number of Data	Data Reference Numbers
		A	B $\times 10^4$	C $\times 10^7$	D						
1	Aziridine	0.805550	-3.51813	3.93398	328.480	0.001*9363.2	175.0*520.0	910.44	0.5580	70	8
2	Azetidine	0.845657	-5.40700	4.84507	333.317	0.016*8539.7	200.0*545.0	715.50	0.2138	70	8
3	Pyrole	0.880256	-6.05913	5.02726	402.916	0.031*6832.3	250.0*635.0	92.813	0.7924	143	8, 24, 39, 35, 51
4	Pyrrolidine	0.917745	-9.28422	8.84658	359.642	0.014*5460.6	215.0*566.5	314.43	0.8259	127	4, 8, 35, 51
5	Pyridine	0.848882	-6.08910	5.15399	388.399	0.029*5645.0	235.0*620.0	140.30	0.7488	181	4, 6, 8, 16, 35, 51
6	1-Methylpyrrole	0.880560	-7.23818	6.44262	375.782	0.016*4790.5	230.0*595.0	151.87	0.3903	100	8, 24, 35
7	Piperidine	0.885414	-7.94176	6.97866	379.377	0.545*4388.7	265.0*590.0	178.96	0.6942	103	8, 16, 35
8	Aniline	0.911551	-6.64936	5.15455	457.025	0.008*5165.0	267.3*695.0	17.520	0.9436	130	4, 6, 8, 16
9	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
10	3-Methylpyridine	0.865977	-6.48542	5.41256	417.217	0.035*4650.0	255.0*645.0	62.139	0.1687	141	4, 8, 16, 35
11	4-Methylpyridine	0.862538	-6.32828	5.24419	418.461	0.284*4548.2	280.0*645.0	59.971	0.1155	115	8, 16, 35
12	2,5-Dimethylpyrrole	0.975279	-8.18064	6.24150	440.662	0.002*5037.7	255.0*660.0	13.262	0.4274	102	8, 35
13	Cyclohexylamine	0.848474	-5.99285	5.24860	406.825	7.843*86.06	333.9*401.5	83.487	0.4113	15	16
14	2-Ethylpyridine	0.890367	-8.35931	7.50471	391.355	0.443*3666.3	270.0*595.0	128.30	0.1978	86	8, 35
15	Benzylamine	0.910765	-6.64743	5.27032	457.650	0.001*4745.4	250.0*685.0	17.106	0.8609	97	8, 41
16	2-Ethylpyridine	0.846505	-5.49471	4.55275	421.790	0.004*3908.4	235.0*630.0	54.072	0.1726	80	8
17	3-Ethylpyridine	0.838237	-5.13221	4.04466	438.545	0.003*3955.2	240.0*660.0	33.524	0.1635	85	8
18	4-Ethylpyridine	0.841038	-5.09376	3.99740	440.104	0.007*3962.8	250.0*660.0	31.753	0.1716	85	8
19	2,3-Dimethylpyridine	0.881714	-6.74484	5.55055	434.216	0.019*4086.3	260.0*655.0	37.695	0.2542	102	8, 16
20	2,4-Dimethylpyridine	0.859213	-5.91288	4.83486	431.576	0.025*3862.5	260.0*645.0	40.741	0.0637	105	8, 16
21	2,5-Dimethylpyridine	0.871144	-6.47984	5.39996	430.124	0.026*3686.8	260.0*640.0	42.629	0.1021	104	8, 16
22	2,6-Dimethylpyridine	0.885281	-7.15067	6.18799	417.136	0.106*3721.5	270.0*620.0	61.925	0.1448	94	8, 16
23	3,4-Dimethylpyridine	0.873502	-6.18582	4.84358	452.235	0.019*3955.1	270.0*680.0	22.173	0.1543	95	4, 8
24	3,5-Dimethylpyridine	0.871062	-6.21188	4.99649	445.022	0.018*3847.1	265.0*665.0	27.435	0.1231	92	4, 8
25	N-Methylaniline	0.921600	-6.99135	5.56325	468.447	0.011*4693.7	280.0*700.0	12.154	0.5250	90	8, 41
26	2-Methylaniline	0.907135	-6.44774	4.94693	473.369	0.049*4649.9	300.0*710.0	10.577	0.2815	90	4, 8
27	3-Methylaniline	0.923479	-6.91988	5.41104	476.329	0.007*4399.1	280.0*705.0	9.4022	0.5243	93	4, 8
28	4-Methylaniline	0.915691	-6.57014	5.11261	473.445	0.020*4443.4	290.0*700.0	10.208	0.3445	97	4, 8
29	2-Methyl-5-vinylpyridine	0.839604	-4.92750	3.78043	455.434	0.027*3650.0	245.0*675.0	20.246	0.3642	88	8
30	N-Ethylaniline	0.918904	-6.84804	5.43030	477.780	0.007*3862.7	280.0*695.0	9.0565	0.3353	84	8
31	4-Ethylaniline	0.912477	-6.54610	5.04275	490.226	0.004*3850.1	280.0*715.0	6.1757	0.3925	88	8
32	N,N-Dimethylaniline	0.909397	-7.07673	5.69581	466.445	0.010*3721.2	275.0*685.0	13.773	0.4667	83	8
33	2,4-Dimethylaniline	0.913798	-6.44268	4.98805	490.122	0.014*3820.3	295.0*710.0	6.0146	0.3603	85	8
34	2,6-Dimethylaniline	0.926009	-6.89676	5.31053	490.795	0.005*4107.4	285.0*720.0	5.9198	0.6847	88	8
35	2-Methyl-5-ethylpyridine	0.845606	-5.35481	4.28671	451.482	0.004*3272.6	250.0*660.0	22.944	0.223	83	8
36	2,4,6-Trimethylpyridine	0.846594	-5.46549	4.48622	443.588	0.006*3200.0	250.0*645.0	28.803	0.221	80	8
37	2-Methyl-4-ethylpyridine	0.807333	-5.47228	4.49971	436.593	0.027*3322.8	260.0*640.0	35.783	0.123	77	8
38	Isoquinoline	0.901210	-6.33869	4.26359	516.182	0.009*4479.0	300.0*800.0	3.1428	0.453	141	4, 8
39	Quinoline	0.897177	-6.73559	4.69707	510.552	0.006*3731.5	290.0*780.0	4.0885	0.520	127	4, 8
40	4-Cunidine	0.884718	-5.66541	5.73271	501.141	0.133*101.3	333.2*500.2	3.9669	0.730	10	41
41	4-Isopropylaniline	0.901277	-6.32720	4.83752	498.038	0.003*3238.6	280.0*715.0	5.0441	0.329	88	8
42	N,N,2-Trimethylaniline	0.890841	-6.76937	5.54004	458.592	0.005*3223.7	339.4*665.0	18.060	0.481	90	8, 41
43	N,N,4-Trimethylaniline	0.924688	-6.88109	5.49146	482.716	0.003*3750.0	275.0*695.0	7.5222	0.424	85	8
44	2,4,5-Trimethylaniline	0.909200	-6.02186	4.52808	507.562	0.154*3500.0	340.0*725.0	3.3522	0.176	78	8
45	3-Methylisouquinoline	0.959525	-7.30332	4.89518	526.133	0.030*4956.9	330.0*805.0	1.7778	0.399	120	4, 8
46	2-Methylisouquinoline	0.936276	-6.69538	4.65103	520.768	0.004*4800.8	300.0*785.0	2.1653	0.352	98	8
47	4-Methylisouquinoline	0.951188	-6.50942	4.37314	538.672	0.010*4554.4	325.0*795.0	1.0167	0.318	95	8
48	6-Methylisouquinoline	0.971408	-7.84250	5.29478	538.063	0.009*3628.2	320.0*795.0	1.2541	0.413	122	4, 8
49	7-Methylisouquinoline	0.942392	-6.45934	4.37190	530.777	0.037*4654.7	330.0*790.0	1.4135	0.278	110	4, 8
50	8-Methylisouquinoline	0.928604	-6.32078	4.26965	520.971	0.006*4950.8	305.0*790.0	2.1283	0.328	115	4, 8
51	1-Naphthylamine	0.822931	-2.94554	2.19845	574.066	0.005*385.56	325.0*645.0	0.40996	0.324	65	8
52	2-Naphthylamine	0.860256	-4.44266	3.1453	579.422	0.161*351.60	385.0*645.0	0.33845	0.307	53	8
53	Quinaldine	0.890722	-6.35906	6.06802	520.647	0.001*101.62	281.9*521.0	2.3606	0.567	50	4, 42
54	N-Diethylaniline	0.923880	-7.08036	5.70974	489.409	0.004*1684.20	280.0*645.0	6.3057	0.286	74	8
55	2,4-Dimethylquinoline	0.981169	-8.10352	5.44560	540.159	0.002*3826.2	305.0*805.0	1.1524	0.705	120	4, 8
56	2,6-Dimethylquinoline	0.962921	-7.46554	4.94350	538.435	0.004*3753.3	310.0*800.0	1.2350	0.443	126	4, 8
57	Carbazol	0.924810	-5.18974	2.68415	627.897	7.333*101.62	518.0*631.0	0.053203 ^c	0.393	42	18, 34
58	Diphenylamine	0.936992	-6.17195	4.32696	575.114	0.005*555.48	335.0*670.0	0.30926	0.582	85	8, 16, 41
59	Acridine	0.839996	-4.19344	3.63487	618.827	0.133*101.33	402.6*619.2	0.11614 ^c	0.920	10	41
60	Methylidiphenylamine	0.913570	-5.42806	5.24849	555.168	0.133*101.33	376.7*555.2	0.46343	0.635	10	41
61	N-Ethylcarbazol	0.906637	-4.74302	5.73341	595.800	0.002*70.015	347.8*373.8	0.071622 ^c	2.04	7	42
62	N-Ethylidiphenylamine	0.910264	-5.67107	3.83118	569.073	0.003*583.05	320.0*670.0	0.45449	0.391	70	8
63	Dibenzylamine	0.924113	-5.87692	4.40076	583.802	0.011*492.57	350.0*670.0	0.23169	0.222	65	8
64	N-Methylidiphenylaniline	0.920504	-5.86374	3.95486	566.122	0.004*623.62	325.0*670.0	0.47251	0.557	70	8

^a P in atm (1.01325 bar or 101.325 kPa); T in K.

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

^c 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	$\log_{10} P = (1-D/T) \times 10^{(A + BT + CT^2)}^a$				Vapor Pressure Range, kPa	Temperature Range, K	Vapor Pressure kPa at 400.0 K	AAD ^b %	Number of Data	Data Reference Numbers
		A	Bx10 ⁴	Cx10 ⁷	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	0.0400	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	Phenylhydrazine	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-Dimethyl-piperazine	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-dimethyl-pyridine	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	376.7~566.2	0.44244	0.461	10	41
15	Di-(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

^a P in atm (1.01325 bar or 101.325 kPa); T in K.

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

^c 400 K outside the temperature range of the data used in evaluating the coefficients of the vapor pressure equation.

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

No.	Name	$\log_{10} P = (1 - D/T)x10^4 (A + BT + CT^2)^a$				Vapor Pressure Range, kPa	Temperature Range, K	AAD ^b %	Number of Data Points	Data Reference Numbers	Calculated Vapor Pressure, kPa, at 400 K
		A	Bx10 ⁴	Cx10 ⁷	D						
1	Furan	0.858331	-8.56435	9.32123	304.367	0.08275500.0	193.15-490.25	0.692	62	4, 14, 51	1291.0
2	Cyclobutanone	0.870584	-9.76474	19.3674	364.075	0.26775.760	249.09-298.39	0.785	11	4	362.52 ^c
3	Tetrahydrofuran	0.830424	-6.81525	6.84786	339.244	1.95475190.0	253.15-540.15	0.612	67	4, 14, 51	515.10
4	2-Methylfuran	0.871223	-7.95690	7.81737	338.704	86.1374722.90	333.45-527.61	0.607	32	24, 51	544.33
5	Cyclopentanone										
6	2-Methyltetrahydrofuran	0.897078	-6.60577	4.52567	359.254	643.373557.7	427.61-533.72	0.477	20	51	333.02 ^c
7	Phenol	1.00375	-8.88757	6.83750	454.610	0.32246132.00	323.20-694.25	1.160	130	2, 4, 6, 11, 16	16.763
8	Cyclohexanone	0.833332	-6.42578	7.09855	428.587	0.1337131.42	274.55-438.92	0.372	26	31, 41	45.267
9	Cyclohexanone	0.951396	-8.46102	8.87926	434.658	0.1337101.33	294.15-434.15	1.032	10	41	32.569
10	2-Hexanone	0.934881	-4.87941	4.16258	400.348	0.1337101.33	280.85-400.65	0.808	10	41	100.03
11	Benzoic Acid										
12	Acisole	0.942238	-10.2065	10.6819	426.827	6.28767.67.661	346.49-415.52	0.123	6	16	46.321
13	Benzylalcohol	1.02742	-6.26739	1.28791	479.624	0.266767.661	340.95-463.65	1.055	18	16	7.4206
14	2-hydroxytoluene(2-cresol)	0.101555	-9.39580	7.92834	463.986	0.12386150.00	313.20-697.65	0.654	120	2, 4, 6, 12, 16	13.137 ^c
15	3-hydroxytoluene(3-cresol)	0.965085	-6.89845	4.47100	475.222	0.002974560.00	278.05-705.85	1.095	110	2, 4, 6, 12, 32, 41	8.3536
16	4-hydroxytoluene(4-cresol)	0.07944	-11.6938	9.28202	475.109	0.11185150.00	323.20-704.65	0.518	123	2, 4, 6, 12, 16	3.4082 ^c
17	Coumarone	0.795901	-4.13024	21.5953	429.907	0.010770.164	273.15-313.15	4.298	7	6	19.856 ^c
18	Acetophenone	0.859974	-6.15392	6.99110	474.823	0.1337101.33	310.25-475.55	1.339	48	16, 41	10.259
19	2-Ethylphenol	0.883881	-6.07675	6.42624	480.731	0.1337101.33	319.35-480.65	0.743	29	4, 41	7.7020
20	3-Ethylphenol	0.971667	-6.29566	2.74908	491.415	0.001733.41	278.11-502.74	1.055	44	4, 15	4.7795
21	4-Ethylphenol										
22	2,3-Dimethylphenol	0.979517	-8.35112	6.60684	489.845	0.30874900.00	343.20-722.95	0.860	110	2, 4, 6, 13, 58	5.4851
23	2,4-Dimethylphenol	0.999891	-8.49456	6.96026	483.891	0.012874400.00	298.02-707.95	0.865	120	2, 4, 6, 13, 58	5.5635
24	2,5-Dimethylphenol	0.993879	-8.99374	7.4099	483.942	0.35974900.00	343.20-707.05	1.175	107	2, 4, 6, 13, 58	5.5604
25	2,6-Dimethylphenol	0.993333	-9.96552	8.34247	474.112	0.100374300.00	312.81-701.05	0.6222	109	2, 4, 6, 13, 58	10.348
26	3,4-Dimethylphenol	1.05062	-10.21229	8.04338	499.926	0.26657000.00	353.20-729.95	0.800	107	2, 4, 6, 13, 58	3.4040
27	3,5-Dimethylphenol	1.04106	-9.50547	6.64831	494.911	0.090173600.00	333.20-715.65	0.338	110	2, 4, 6, 13, 58	4.1444
28	5-Indanol										
29	2-Ethylanisole	0.881926	-6.65998	7.00344	460.386	0.1337101.33	302.85-460.25	0.554	10	41	15.830
30	3-Ethylanisole	0.874023	-6.87264	7.50986	469.810	0.1337101.33	306.85-469.65	0.620	10	41	12.340
31	4-Ethylanisole	0.872105	-6.70633	7.23277	469.450	0.1337101.33	306.65-469.65	0.700	10	41	12.457
32	3-Methyl-5-ethylphenol	0.913828	-6.36557	7.26448	505.528	1.3337101.33	384.65-506.15	1.128	19	4	2.7081
33	2-Isopropylphenol	0.912522	-6.17902	6.51481	487.650	0.1337101.33	329.75-487.65	0.679	10	41	5.2072
34	3-Isopropylphenol	0.901582	-6.42031	6.19158	501.397	0.1337101.33	335.15-501.15	0.738	10	41	3.6502
35	4-Isopropylphenol	0.932791	-6.98250	7.55366	501.658	0.1337101.33	340.15-501.35	0.777	10	41	3.1199
36	3-Phenyl-1-propanol	0.934132	-6.11678	6.13688	508.280	0.1337101.33	347.85-508.15	0.929	10	41	2.2162 ^c
37	2-Propylphenol	0.875307	-5.52137	7.84123	494.836	6.6667101.33	414.45-494.65	0.841	17	4	3.7792 ^c
38	4-Propylphenol	0.733568	-5.59797	13.8634	506.814	9.9997101.33	428.35-507.65	1.537	16	4	3.6892 ^c
39	2,3,5-Trimethylphenol	0.932965	-5.75276	3.29737	508.477	26.5477133.34	459.63-520.21	0.007	17	4	2.8897 ^c
40	4-Isobutylphenol										
41	1-Hydroxynaphthalene	0.881442	-5.80731	6.06214	555.113	0.1337101.33	367.15-555.95	1.181	38	4, 6	0.69877
42	2-Hydroxynaphthalene	0.874875	-5.63554	5.87458	560.208	0.6677101.33	401.75-561.15	1.181	27	4, 6	0.61258 ^c
43											
44	4-sec-Butylphenol	0.885386	-5.26451	5.13029	515.194	0.1337101.33	344.55-515.25	0.522	10	41	2.2928
45	2-tert-Butylphenol	0.898200	-6.62186	5.90279	497.209	6.8857104.958	407.80-498.58	0.261	8	4	5.0968 ^c
46	4-tert-Butylphenol	0.834403	-2.10918	0.554077	512.693	0.1307133.35	343.15-524.76	1.159	26	4, 41	2.4469
47	3,5-Diethylphenol	0.876394	-6.55074	7.65283	521.080	1.3337101.33	387.65-521.15	0.963	19	4	2.2617
48	4-(1,1,3,3-Tetramethyl)Phenol	0.967228	-6.46884	3.61657	563.562	8.7077103.87	472.47-564.77	0.097	9	4	0.41506 ^c
49	2-tert-Butyl-4-Cresol	0.915488	-6.16723	6.81023	505.681	0.1337101.33	343.15-505.75	0.615	10	41	2.6419
50	4-tert-Butyl-2-Cresol	0.889494	-5.55746	5.24049	519.836	0.1337101.33	347.45-520.15	0.530	10	41	1.9869
51	2-Phenylphenol	0.889463	-4.72320	5.27654	549.249	0.1337101.33	373.15-548.15	1.672	28	4, 41	0.53903
52	4-Phenylphenol	0.949514	-5.54686	5.61184	580.171	1.3337101.33	450.15-581.15	0.891	19	4	0.11152 ^c
53											
54	2-tert-Butyl-4-ethylphenol	0.893089	-6.11822	7.45086	520.515	0.1337101.33	349.45-520.95	0.914	10	41	1.7438
55	4-tert-Butyl-2,4-xylenol	0.878041	-5.47812	6.92216	538.275	0.1337101.33	361.35-538.45	1.968	10	41	0.93692
56	4-tert-Butyl-2,6-xylenol	0.871204	-5.99541	9.85796	512.389	0.1337101.33	347.15-512.95	1.513	10	41	1.8914
57	6-tert-Butyl-2,4-xylenol	0.873072	-6.06053	9.46410	509.117	0.1337101.33	343.45-509.65	1.182	10	41	2.2600
58	6-tert-Butyl-3,4-xylenol	0.916526	-5.81421	6.69496	522.451	0.1337101.33	357.05-522.65	0.748	10	41	1.2986
59	2,4-Diisopropylphenol	0.916060	-6.48571	5.72246	527.384	1.3337101.33	395.15-528.15	1.665	19	4	1.6685
60	2-Phenylethylphenol	1.23153	-8.10573	-10.1736	637.998	0.813718.78	442.35-523.45	1.852	29	4	0.05032 ^c
61	4-Phenylethylphenol	1.25864	-8.45954	-10.7815	664.652	0.560713.18	447.55-523.65	1.917	23	4	0.02015 ^c

^a P in atm (1.01325 bar or 101.325 kPa); T in K.

^b ADD = absolute average deviation.

^c 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	$\log_{10} P = (1-D/T) \times 10^4 (A + BT + CT^2)^a$	Vapor Pressure Range, kPa	Temperature Range, K	ΔD^b	No. of Data Points	Data Reference Numbers	Calculated Vapor Pressure, kPa, at 400 K
		A	$B \times 10^4$	$C \times 10^7$	D			
1	Quinone (9-Benzoquinone)	0.902426	-6.04783	6.58278	517.477	0.6677101.33	377.15 ¹ 518.65	1.9583
2	1,2-Dihydroxybenzene	0.958295	-5.78954	5.46841	549.041	0.1337101.33	381.55 ¹ 549.65	0.37720
3	1,3-Dihydroxybenzene	0.941185	-5.32724	5.41185	558.031	1.3337101.33	432.25 ¹ 559.15	0.28743
4	Pyrogallol	0.935304	-5.49471	6.15169	580.441	1.3337101.33	450.45 ¹ 582.15	0.11370
5	Quinacrol	0.858892	-4.47192	3.22549	477.010	1.3337101.33	355.15 ¹ 478.15	9.2881
6	Di phenylene Oxide							
7	Dibenzofuran	0.872631	-6.33808	7.42629	596.940	1.3337101.33	444.15 ¹ 598.15	0.809
8	2,2'-Diphenol							
9	Quinhydrone							
10	Anthanthrone							
11								0.20547

a P in atm (1.01325 bar or 101.325 kPa); T in K.

b ADD = absolute average deviation.

c 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 ΔH_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 reliability²⁰ which is the main purpose of this work.

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