



An easily applied method for predicting binary gas-phase diffusivities is based on the use of special diffusion volumes coupled with extensive experiment and nonlinear least squares analysis of the data. Comparison with eight other correlations demonstrates the relative reliability and simplicity of the new method.

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A NEW METHOD FOR PREDICTION OF BINARY GAS-PHASE DIFFUSION COEFFICIENTS

The importance of gaseous diffusion in a wide variety of chemical processes is well known. With growing demands for the quantitative description of these processes and with recent advances in mass transport theory, there has been an increasing need for accurate gas-phase diffusion coefficients for reference purposes. As a result of the scarcity of reliable experimental data, methods for estimating diffusion coefficients must frequently be employed to meet the need. A number of such methods have been reviewed elsewhere (11, 15, 44).

The present investigation develops a simple, reliable, and widely applicable correlation equation for the estimation of gas-phase diffusion coefficients. This approach starts with the Stefan-Maxwell hard sphere model and the principle of additive atomic volumes first employed in estimating diffusion coefficients by Arnold (5) and Gilliland (18). Selected "constants" are allowed to

vary freely, with optimum values obtained from a nonlinear least squares analysis involving, in this case, 340 experimental diffusion coefficients obtained from the literature.

A detailed comparison of the final equation has been made with the methods of Arnold (5), Gilliland (18), Hirschfelder-Bird-Spotz (20-22), both original and as modified by Wilke and Lee (64), Andrusow (4), Slattery Bird (54), Chen-Othmer (11), and Othmer-Chen (41) on all 340 data points. The present correlation has proved to be quite accurate, more so than all others for the 340 reference points. Despite the large sample, this is not a totally objective test since the parameters were obtained from these particular data. This method shows the added advantage of being simpler to apply than the more rigorous techniques.

The large collection of diffusion data assembled in this report should prove useful to the many workers interested in gas-phase diffusion.

Theory

The origin of most empirical diffusion correlations can be traced back to the hard sphere model, given below in

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the Chapman-Enskog form (9)

$$D_{AB} = \frac{3}{32n\sigma_{AB}^2} \left[\frac{8kT}{\pi} (1/m_A + 1/m_B) \right]^{1/2} \quad (1)$$

- D_{AB} = binary diffusion coefficient, sq. cm./sec.
 n = total concentration of both species, molecules/cc.
 T = temperature, ° K.
 k = the Boltzmann constant, ergs/° K.
 m_A, m_B = molecular mass, grams
 σ_{AB} = $1/2 (\sigma_A + \sigma_B)$, collision diameter, separation between molecular centers of unlike pairs upon collision, cm.

This equation is sometimes used to predict gaseous diffusion coefficients, but its use suffers from two serious limitations. The first limitation is the $^{3/2}$ power temperature dependence; observed values usually lie in the range 1.6 to 1.8 (29, 53). This difference between the simple theory and experimental observations arises from the fact that σ slowly decreases with increasing temperature (molecular softness). The second limitation, although not a source of error, is that very few of the required σ are available in the literature, and even these are applicable only over narrow temperature ranges because of the temperature dependence of σ .

In 1930 Arnold (5) made two contributions aimed at overcoming the two main limitations on the hard sphere model. First he introduced a Sutherland temperature correction in his equation to obtain an improved temperature dependence. In addition, he correlated σ with an easily measured property of the diffusing substance; in his method, σ was estimated as the cube root of the sum of Le Bas atomic volume parameters. Arnold's second contribution solved the problem stemming from the scarcity of experimental σ 's, making it possible to estimate diffusion coefficients for almost any binary gas phase system.

The correlation of σ with molar boiling point volumes estimated from the Le Bas parameters was retained by Gilliland (18) in his correlation of 1934, but he eliminated the Sutherland temperature correction. An apparent explanation for this step was increased simplicity. Lack of data for diffusion coefficients as a function of temperature with which to check the Arnold correction made the latter doubtful in value.

Other workers have pursued different lines of attack. In 1950 another correlation based on the Le Bas parameters was introduced by Andrusow (4) with a 1.78 power temperature dependence. Some workers have estimated σ from the cube root of the critical volume, and in 1962 Chen and Othmer (7) used the 0.4 power of the critical volume. Correlations based on critical volumes, however, are only partially able to overcome the second limitation of the hard sphere model since experimental critical volumes have been determined for only a limited number of substances.

To gain even more freedom from the physical and mathematical restrictions of the hard sphere model, the following generalized function was fitted to the data in this investigation:

$$D_{AB} = \frac{CT^{\beta}(1/M_A + 1/M_B)^{1/2}}{p[(\Sigma_A v_i^{\alpha_1} + \Sigma_B v_i^{\alpha_2})^{\alpha_3}]} \quad (2)$$

C = an arbitrary constant

p = pressure, atm.

M_A, M_B = mol. wt., gram/mole

The parameters listed below are to be optimized by least squares analysis:

b = temperature power dependence

v_i = special diffusion parameters to be summed over atoms, groups, and structural features of the diffusing species (dimensions determined by the α 's)

$\alpha_1, \alpha_2, \alpha_3$ = arbitrary exponents to the $\Sigma_A v_i$ and $\Sigma_B v_i$

Later the v_i 's will be converted to "diffusion volumes," but in this general form these are simply general parameters for which an additive relationship has been assumed. The procedure for estimating σ by means of additive diffusion parameters is analogous to the procedure used in the earlier Arnold method using the Le Bas volumes. However, the present approach of using parameters obtained directly from experimental diffusion data probably has a higher accuracy than methods using parameters obtained by independent means.

All parameters for use in the present correlation were obtained from a nonlinear least squares analysis of 153 different binary systems (340 actual data points). The resulting fit to these data gave an average difference between observed and predicted values of only 4.3%.

The Computational Problem

The least squares analysis involved minimizing the expression:

$$\phi' = \sum_{i=1}^N [Y_i - E_i/Y_i]^2 \quad (3)$$

ϕ' = sum of the squares of the relative differences between observed and estimated values

N = number of data points

Y_i = i^{th} observed value of the dependent variable; in this case the observed D_{AB}

E_i = i^{th} estimated value corresponding to Y_i ; in this case D_{AB} estimated from Equation 2

The relative least squares approach was used because the experimental values range over three orders of magnitude while the fractional experimental error probably remains almost constant. In such cases an absolute least squares analysis becomes dominated by the larger diffusion coefficients and their corresponding larger absolute deviations.

An excellent general Fortran program by Marquardt (39) [see also references (37, 38)] was easily adapted to the solution of this rather formidable problem of minimizing the ϕ' function simultaneously with respect to all the parameters. When we started with initial guesses for the volume parameters obtained from scaled critical

volumes and reasonable values for the others, the IBM 7040 computer met the convergence tests of the program by means of iteration over different values of each parameter in roughly $1/2$ hour of operation.

Results and Discussion

The final equation selected from the least squares studies is given by

$$D_{AB} = \frac{1.00 \times 10^{-8} T^{1.75} (1/M_A + 1/M_B)^{1/2}}{p[(\sum_A v_i)^{1/3} + (\sum_B v_i)^{1/3}]^2} \quad (4)$$

The high degree of correlation between α_1 , α_2 , α_3 , and the v_i 's and the nearness of the α 's to the hard sphere values led us to try the latter in Equation 2. Thus, Equation 4 was obtained from Equation 2 by arbitrarily using the values $\alpha_1 = \alpha_2 = 1/3$ and $\alpha_3 = 2$. Consequently, the simple form, above, was retained. The v 's now have the dimensions of atomic volumes and will be referred to as "diffusion volumes."

The 1.75 temperature power dependence represents a compromise value giving reasonable agreement for most binary systems. The actual value of b obtained from the least squares analysis was $b = 1.749 \pm 0.013$ (approximate 95% confidence limits). The value of b was then rounded to 1.75 for the sake of simplicity; inasmuch as Equation 2 is sensitive to small changes in b , it was necessary to run the least squares program once more for the purpose of adjusting the remaining parameters to minimize ϕ' with b constrained to this value (ϕ' at least squares minimum = 1.4707, at the constrained minimum = 1.4762). The resulting small increase in ϕ' was taken to be insignificant.

The initial arbitrary constant, C , was chosen as 1.00×10^{-8} . This value was picked so that the atomic diffusion volumes would roughly correspond to Le Bas volumes. With this constant, diffusion volumes are usually about 10 to 15% smaller than the Le Bas volume. The resulting optimized values of the special diffusion

volumes are listed in Table I. In the upper part of the table are listed the diffusion volume increments to be summed when applying the method to organic vapors other than simple gases (such as N_2 , CO_2 , ...). The Σv values for the simple gases are listed in the lower part. The use of a single parameter for these gases results in improved accuracy although it would be possible to estimate these volumes by summing increments as before. This approach stems from the fact that, in general, typical organic substances tend to obey additivity relations much better than substances such as those listed in the lower part.

Thus far, the special atomic diffusion volumes have not been determined for —F, —Br, and —I because data for compounds containing these constituents do not appear to be available. Experimental diffusion data to determine these unknown increments and additional data for those increments based on only a few points

TABLE I. SPECIAL ATOMIC DIFFUSION VOLUMES^a

Atomic and Structural Diffusion Volume Increments			
C	16.5	(Cl)	19.5
H	1.98	(S)	17.0
O	5.48	Aromatic or Hetero-	
(N) ^b	5.69	cyclic rings	-20.2
Diffusion Volumes of Simple Molecules			
H_2	7.07	CO_2	26.9
D_2	6.70	N_2O	35.9
He	2.88	NH_3	14.9
N_2	17.9	H_2O	12.7
O_2	16.6	(CCl_2F_2)	114.8
Air	20.1	(SF_6)	69.7
Ne	5.59		
Ar	16.1	(Cl_2)	37.7
Kr	22.8	(Br_2)	67.2
(Xe)	37.9	(SO_2)	41.1
CO	18.9		

^a $b = 1.75$.

^b () indicates that listed value is based on only a few data points.

TABLE II. SUMMARY OF RESULTS^a

System Type	No. of Exptl. Points	Category I Methods				Category II Methods				
		FSG	Gilliland	Andrusow	Arnold	HBS	Mod. HBS, Wilke-Lee	Chen, Othmer	Slattery, Bird	Othmer, Chen
H_2	59	5.8	14.0	10.1	24.8	8.3	8.7	6.8	14.7	9.7
He	108	3.9	32.8	23.8	7.6	5.9	6.3	14.1	26.1	22.7
N_2	71	3.8	24.3	18.4	8.5	5.7	6.8	7.0	9.1	10.6
O_2	23	2.3	20.6	16.1	5.0	5.4	2.6	11.0	9.0	15.9
Ar	58	3.3	28.8	25.8	8.5	4.2	5.7	8.5	8.2	12.3
Air	53	5.7	14.2	12.4	6.6	6.3	8.0	7.6	8.6	8.2
NH_3 , H_2O	41	4.4	21.2	14.2	13.7	6.0	7.2	10.0	27.1	13.6
Organic substances	154	5.0	14.9	11.3	10.9	8.3	8.1	8.3	14.3	15.2
Overall % error	340	4.3	21.1	16.6	10.7	6.4	6.8	8.9	14.0	
						(5.4) ^b	(5.6) ^b		(6.2) ^c	13.9
						(8.9) ^d	(10.1) ^d			
Per cent of calculated values with more than 10% error		7.4	79.8	74.4	37.1	19.1	20.6	40.0	45.9	55.3

^a All entries are in average % error except as noted. ^b Average % error excluding starred systems. ^c Average % error excluding H_2 and He systems. The error from H_2 and He estimates should not be charged to the Slattery-Bird method since the method does not apply to these systems. ^d Average % error for starred system in Table III.

would be valuable in extending the range and accuracy of the present method.

Certain structural features make contributions to the diffusion volume. A value has been determined for the aromatic ring (which has been grouped with heterocyclic rings) to be subtracted from the usual diffusion volume to account for the bond shortening observed for this type of molecular structure. With further refinements, branched chain, double bond, and triple bond effects should also be taken into account; this is not now worthwhile with the limited accuracy and number of data points available. These effects are apparently smaller than those of an aromatic ring, and for the double and triple bonds are already partially accounted for by adding in the smaller number of —H volume increments.

Equation 4 together with the atomic diffusion volumes listed in Table I provides a simple method for estimating binary gaseous diffusion coefficients. No additional data are required for its use and on the basis of the comparison which follows it is seen to be reliable for a wide variety of systems. As additional experimental data become available, other atomic diffusion volumes can be determined and possibly minor adjustments made in the ones already listed to improve the method.

Comparison of Methods

For the purpose of this report methods for estimating D_{AB} will be grouped into two broad categories. The first category includes the present correlation and those procedures like the Gilliland method which consist of an equation and a limited set of atomic and structural parameters. These methods require no supplementary data and are thus applicable to a wide range of substances. The second category includes methods such as the Hirschfelder-Bird-Spotz equation which relate diffusion to various molecular properties and thus require extensive data, such as knowledge of intermolecular forces or of critical properties covering every different substance for which the calculations are to be made. The requirement for considerable supplemental data seriously restricts the range of applicability of category two methods since the required data are, in most cases, available for only a limited number of common substances. Category one methods are usually easier to apply and are applicable to a wider range of compounds than category two methods, but lack of rigor reduces the accuracy as will be seen shortly.

Before comparing the various methods, some comments about the experimental data are desirable. First it should be pointed out that accurate experimental diffusion measurements are difficult to make and that most observations are subject to a fair amount of experimental uncertainty; this difficulty is greatest for high molecular weight compounds. The typical amount of error is probably of the order of 5%, as can be seen from the fact that observations reported in the literature for identical systems often differ by this amount or more. A second limitation on the experimental side is that diffusion data, in particular for organic vapors, are quite limited in

scope both as to types of systems and the range of temperatures. As a result, even considering all available data, no completely adequate test of correlation methods appears possible.

The list of experimental data in Table III, although extensive, is by no means complete. Several additional sources might have been included but were either not available or unknown to the authors during the period in which the bulk of this study was carried out [see for example references (8, 33, 36, 42, 45, 46, 55, 58, 63)]. No doubt other sources have been overlooked. For the purposes of this investigation, only recent determinations (no data before 1930 being included) were considered; since, as pointed out by Scott (52), much of the early work requires critical evaluation.

Eight methods, in addition to the present one, are compared by calculating values of the diffusion coefficient for all the experimental points used in fixing parameters for the present correlation. The results of these calculations are listed in Table II. To conserve space, only per cent error has been given where

$$\% \text{ error} = \frac{D_{\text{calcd.}} - D_{\text{obsd.}}}{D_{\text{obsd.}}} \times 100 \quad (5)$$

If desired, any calculated D_{AB} value can be obtained by use of the above equation.

For those methods based mainly on Le Bas molar boiling point volumes—the Arnold, Gilliland, and Andrusow methods—the values of parameters listed in Arnold's paper (5) were used in the calculations. For the noble gases, experimental boiling point volumes, V_b , were used except for helium and neon which have abnormally large V_b values. Much better results were obtained with these correlations using values ($V_{bHe} = 7.21$; $V_{bNe} = 12.9$) estimated from viscosity data according to an equation given by Arnold (5). Sutherland constants for use in the Arnold method were taken from reference (10); all others not listed there were estimated by a relation used by Arnold:

$$C = 1.47 T_b \\ T_b = \text{boiling point temperature, } ^\circ\text{K.} \quad (6)$$

For methods employing collision integrals, the Hirschfelder-Bird-Spotz method (hereafter referred to as the HBS method), and the Wilke-Lee modification of the HBS method, the required force constants were taken from the literature (22) and (23). Svehla (59) has published a more extended list with some values slightly different from those in the literature (22) and (23). These parameters have been determined for most light gases and a limited number of organic vapors.

All starred points in Table III indicate that these parameters were not available for one or both of the components and were estimated from critical properties. In calculations using these methods no corrections for polarity were made nor were higher approximations taken. Undoubtedly somewhat better agreement between estimated and observed results could have been

achieved using these refinements; however, this would have involved a substantial increase in labor.

All critical data for the correlations requiring them were taken from reference (32) (except for V_c of D_2 which was taken from reference (24) since the value quoted in (32) is in error). In some cases, critical data for some of the organic vapors were not available—the required data were estimated using the methods due to Lydersen (35) as quoted by Reid and Sherwood (43).

Data for the viscosity of air as a function of temperature, required for the Othmer-Chen reference substance method, were taken from a National Bureau of Standards circular (40).

The results of the comparison are displayed in Table III and have been summarized in Table II. The Gilliland method is found to be the most erratic, showing an overall 21.1% average error, with the closely related Andrusow correlation performing slightly better. The

TABLE III. PERCENTAGE ERROR INTRODUCED BY VARIOUS EQUATIONS
USED TO PREDICT EXPERIMENTAL DIFFUSION COEFFICIENTS.

SYSTEM	REF.	TEMP. ^a	OBS. ^b	FSG ^c	ANDR ^d	HBS ^e	CH-OT ^f	OT-CH ^g	GILL ^h	ARN ⁱ	MOD-HBS ^j	SL-BDK ^k
H ₂ -HE	17	298.2	1.1320	46.16	12.18	44.36	74.52	37.94	27.34	54.66	61.52	43.40
H ₂ -D ₂	19	288.2	1.2400	-2.99	-3.52	22.98	50.30	-5.67	-12.93	-1.25	0.33	-14.14
H ₂ -D ₂	27	295.5	1.2500	0.54	-0.64	27.55	55.57	-2.21	-9.73	2.49	4.17	-10.19
H ₂ -N ₂	47	193.0	0.3680	-3.72	-12.06	-15.83	19.05	-2.16	-6.20	-2.44	-3.24	-22.02
H ₂ -N ₂	48	200.0	0.4010	-5.96	-14.86	-17.70	16.49	-4.43	-8.38	-4.51	-5.24	-22.17
H ₂ -N ₂	47	253.0	0.6000	-5.16	-19.04	-16.42	18.12	-3.96	-7.93	-2.33	-2.79	-11.26
H ₂ -N ₂	47	273.0	0.7080	-8.19	-23.10	-18.90	14.30	-7.69	-11.50	-5.01	-5.36	-11.22
H ₂ -N ₂	6	287.5	0.7430	-4.22	-20.81	-15.26	19.13	-3.48	-7.47	-0.60	-0.90	-5.48
H ₂ -N ₂	52	294.0	0.7630	-3.01	-20.25	-14.13	20.57	-2.35	-6.39	0.79	0.52	-3.48
H ₂ -N ₂	17	297.2	0.7790	-3.18	-20.61	-14.26	20.31	-2.58	-6.61	0.68	0.42	-3.27
H ₂ -N ₂	48	300.0	0.8000	-4.16	-21.60	-15.10	19.06	-3.76	-7.74	-0.29	-0.53	-3.93
H ₂ -N ₂	47	303.5	0.8520	-8.17	-25.09	-18.62	14.05	-7.72	-11.53	-4.39	-4.61	-7.56
H ₂ -N ₂	52	322.0	0.9030	-3.90	-22.77	-14.69	19.08	-3.80	-7.77	0.41	0.26	-1.33
H ₂ -N ₂	52	398.0	1.2890	-2.46	-25.65	-12.86	19.38	-3.52	-7.51	3.22	3.35	5.97
H ₂ -N ₂	49	400.0	1.2700	-0.12	-23.97	-10.76	22.18	-1.25	-5.33	5.72	5.86	8.62
H ₂ -N ₂	52	450.0	1.5410	1.15	-25.23	-9.30	22.53	-0.84	-4.94	7.83	8.14	12.44
H ₂ -N ₂	52	506.0	1.8830	1.64	-27.04	-8.54	21.69	-1.21	-5.30	9.12	9.60	14.79
H ₂ -AR	52	573.0	2.4170	-1.56	-31.50	-11.09	16.19	-5.00	-8.93	6.47	7.11	12.37
H ₂ -AR	57	287.9	0.8280	-11.19	-27.05	-23.77	4.71	-9.75	-13.30	-6.89	-8.95	-7.78
H ₂ -AR	57	354.2	1.1110	-4.87	-25.81	-17.84	12.00	-4.16	-7.93	0.97	-0.99	5.64
H ₂ -AR	57	418.0	1.7140	-17.61	-38.35	-28.49	-3.63	-17.67	-20.91	-11.67	-13.21	-4.93
H ₂ -CO	27	295.6	0.7430	-1.53	-15.63	-9.02	27.53	2.10	-2.12	2.32	2.58	-1.45
H ₂ -CO ₂	6	289.2	0.6190	-2.34	-8.59	-4.93	25.99	-3.06	-6.84	3.37	-0.42	10.66
H ₂ -CO ₂	7	298.0	0.6460	-1.38	-8.38	-3.91	27.37	-2.40	-6.20	4.57	0.78	12.99
H ₂ -CO ₂	17	298.2	0.6650	-4.08	-10.91	-6.54	23.88	-4.84	-8.55	1.71	-1.98	9.92
H ₂ -WATER	50	307.3	1.0200	-9.19	-19.90	-9.65	-4.02	-4.26	-8.56	-19.76	33.40	2.85
H ₂ -WATER	50	328.6	1.1210	-7.09	-19.41	-7.38	-0.96	-1.66	-6.08	-17.57	41.93	7.56
H ₂ -WATER	50	352.7	1.2000	-1.76	-16.28	-1.86	5.54	3.97	0.69	-12.48	56.41	16.09
H ₂ -NH ₃	52	273.0	0.7454	-4.50	-20.50	-12.85	-1.00	9.09	4.13	-14.36	-23.11	-3.23
H ₂ -NH ₃	52	293.0	0.8337	-3.37	-20.97	-11.63	0.90	10.84	5.81	-12.98	-21.79	0.64
H ₂ -NH ₃	27	296.8	0.8560	-3.74	-21.53	-11.94	0.63	10.54	5.51	-13.24	-22.02	0.73
H ₂ -NH ₃	52	333.0	1.0210	-1.29	-21.81	-9.38	4.13	13.36	8.20	-10.42	-19.36	7.32
H ₂ -NH ₃	52	413.0	1.4350	2.37	-23.16	-5.41	9.00	17.79	12.44	-5.89	-15.05	17.43
H ₂ -NH ₃	52	533.0	2.1490	6.82	-24.78	-0.55	13.65	22.02	16.47	-0.28	-9.69	27.08
H ₂ -SF ₆	57	286.2	0.3960	-2.07	-3.56	-5.68	32.66	-2.28	-5.80	11.30	17.33	10.36
H ₂ -SF ₆	57	306.9	0.4580	-4.32	-7.41	-7.65	29.94	-4.30	-7.75	9.20	15.22	10.59
H ₂ -SF ₆	57	370.8	0.6470	-5.70	-12.95	-8.46	28.33	-6.00	-9.38	8.86	15.14	15.28
H ₂ -SF ₆	57	418.0	0.8380	-10.21	-19.56	-12.53	21.93	-10.87	-14.08	4.40	10.60	12.70
H ₂ -METHANE	7	298.0	0.7260	-5.33	-10.44	1.12	27.25	-1.14	-5.70	0.77	0.29	2.34
H ₂ -ETHANE	7	298.0	0.5370	-3.33	-6.99	0.02	29.24	3.18	-1.04	3.65	6.46	7.20
H ₂ -N-BUTANE	57	287.9	0.3610	-0.34	-2.26	-0.11	31.04	12.18	7.92	4.53	14.36	5.05
H ₂ -N-BUTANE	57	354.2	0.5070	1.99	-5.03	2.85	35.20	15.97	11.57	8.30	18.81	14.98
H ₂ -N-BUTANE	57	430.0	0.7630	-4.85	-15.59	-3.48	26.14	8.51	4.40	2.23	12.43	12.05
H ₂ -N-HEXANE	14	288.7	0.2900	3.08	1.41	1.66	34.72	12.12	7.98	4.82	20.84	3.33
H ₂ -2,3-DIMETHYLBUTANE*	14	288.8	0.3010	-0.63	-2.25	-2.00	30.54	9.44	5.40	2.76	18.67	1.44
H ₂ -CYCLOXANE	14	288.5	0.3190	-4.94	0.14	0.48	30.60	1.51	-2.24	3.31	15.94	5.30
H ₂ -METHYLCYCLOPENTANE*	14	288.5	0.3180	-4.64	-0.94	-0.60	30.05	7.75	3.77	2.29	15.84	3.28
H ₂ -N-PENTANE*	12	303.2	0.2830	6.85	3.95	4.92	39.91	15.89	11.65	7.37	26.74	6.38
H ₂ -2,4-DIMETHYLPHENATE*	12	303.3	0.2970	1.87	-0.90	0.04	34.41	11.87	7.77	3.84	23.71	2.57
H ₂ -N-OCTANE	12	303.2	0.2770	2.27	-0.42	-0.05	33.85	-3.74	-7.24	0.71	22.15	-1.25
H ₂ -2,2,4-TRIMETHYLPHENATE*	12	303.2	0.2920	-2.98	-5.53	-5.18	28.31	7.11	3.21	-1.61	19.78	-3.64
H ₂ -N-DECANE*	14	364.1	0.3060	6.32	11.35	50.57	25.12	20.61	13.10	40.84	14.32	
H ₂ -2,3,3-TRIMETHYLHEPTA*	14	363.9	0.2700	29.26	20.40	26.07	70.86	41.68	36.58	28.05	59.46	29.41
H ₂ -N-DODECANE*	14	399.6	0.3080	21.74	10.81	18.34	60.90	33.99	29.19	19.39	53.26	20.97
H ₂ -BENZENE	26	311.3	0.4036	-0.82	-2.03	0.77	29.21	6.41	2.46	2.10	11.54	8.88
H ₂ -PYRIDINE*	26	317.9	0.4370	1.94	-3.54	-0.26	25.55	0.17	-3.54	-2.78	9.58	5.79
H ₂ -PIPERIDINE*	26	314.7	0.4030	-7.67	-7.24	-4.69	22.59	2.11	-1.66	-2.05	9.82	4.10
H ₂ -THIOPHENE*	26	302.2	0.4000	6.46	-1.69	-0.06	27.46	4.89	1.01	2.39	3.56	10.38
H ₂ -TETRAHYDROTHIOPHENE*	26	318.4	0.4120	-3.08	-4.05	-1.25	27.38	5.03	1.16	1.81	9.12	10.79
D ₂ -HE	27	295.1	1.2500	8.60	-18.13	1.01	27.25	-1.02	-4.53	13.69	18.91	3.11
D ₂ -N ₂	27	296.8	0.5420	3.31	-16.53	-10.32	26.46	1.06	2.09	6.64	6.82	-2.09
D ₂ -AIR	27	296.8	0.5650	-5.48	-18.46	-12.59	23.83	-1.98	-0.94	3.19	2.82	-4.33
D ₂ -AR	27	296.8	0.5750	-0.48	-20.12	-16.06	15.58	-1.83	-0.56	3.85	1.91	-0.91
D ₂ -CO	27	295.7	0.5490	-0.79	-16.26	-10.13	26.59	-0.03	0.99	2.34	3.07	-5.76
D ₂ -CO ₂	27	295.7	0.4740	-2.51	-10.51	-6.60	24.14	-5.87	-4.60	2.67	-0.61	5.53
D ₂ -NH ₃	27	296.8	0.6300	-0.90	-20.46	-11.54	2.00	10.24	10.75	-11.26	-20.00	-1.07
D ₂ -SF ₆	27	295.7	0.3050	-2.69	-6.02	-7.29	30.50	-34.00	-32.84	9.93	16.95	4.55
D ₂ -N-HEPTANE*	12	303.2	0.2180	0.37	-3.27	-2.45	30.19	6.53	8.32	-0.19	19.37	-6.13
D ₂ -2,4-DIMETHYLPHENATE*	12	303.2	0.2240	-2.32	-5.86	-5.07	27.66	4.98	6.74	-1.46	18.93	-7.62
D ₂ -N-OCTANE	12	303.2	0.2080	-1.59	-5.05	-4.77	27.62	-9.18	-7.62	-4.13	17.89	-10.82
D ₂ -2,2,4-TRIMETHYLPHENATE*	12	303.2	0.2120	-3.44	-6.84	-6.57	26.53	4.27	6.05	-3.12	19.56	-9.97
HE-N ₂	59	293.0	0.7050	-3.58	-36.66	-32.20	-5.14	-3.52	-2.52	7.52	10.77	3.73
HE-N ₂	60	298.0	0.7300	-4.08	-37.26	-32.52	-5.67	-4.14	-3.16	7.07	10.33	3.83
HE-N ₂ (TR)	60	298.0	0.6880	1.77	-33.43	-28.40	0.09	1.71	2.75	13.60	17.06	10.17
HE-N ₂ (TR)	17	298.2	0.6870	2.04	-33.26	-28.21	0.35	1.96	3.01	13.91	17.37	10.48
HE-N ₂ (TR)	17	298.2	0.7170	-2.23	-36.06	-31.21	-3.84	-2.31	-1.30	9.14	12.46	5.86
HE-N ₂	60	300.0	0.7430	-4.65	-37.73	-32.90	-6.24	-4.78	-3.80	6.47	9.73	3.46

SYSTEM	REF.	TEMP. ^a	OBS. ^b	FSG ^c	ANDR ^d	HBS ^e	CH-OT ^f	OT-CH ^g	GILL ^h	ARN ⁱ	MOD-HBS ^j	SL-BD ^k
HE-N2	53	323.2	0.7660	5.36	-32.46	-25.69	3.38	4.30	5.37	18.18	21.91	17.24
HE-N2	53	353.2	0.8930	5.57	-33.82	-25.35	3.17	3.20	4.26	19.04	22.94	20.58
HE-N2	53	383.2	1.0770	0.95	-37.99	-28.43	-1.79	-2.26	-1.25	14.40	18.27	17.71
HE-N2	53	413.2	1.2000	3.38	-37.68	-26.55	0.04	-0.70	0.32	17.68	21.78	22.51
HE-N2	53	443.2	1.2890	8.80	-35.55	-22.53	4.70	3.82	4.89	24.38	28.83	30.59
HE-N2	53	473.2	1.5690	0.24	-41.59	-28.49	-4.10	-4.82	-3.85	15.04	19.26	21.52
HE-N2	53	498.2	1.6500	4.31	-40.00	-25.47	-0.70	-1.36	-0.34	20.08	24.56	27.28
HE-N2	60	600.0	2.4000	-0.71	-45.48	-28.66	-7.42	-6.90	-5.94	15.58	20.19	22.99
HE-N2	60	900.0	4.7600	1.78	-49.50	-25.98	-10.43	-8.05	-7.10	21.40	26.91	25.03
HE-N2	60	1200.0	7.7400	3.55	-52.18	-24.03	-13.27	-8.93	-7.99	25.67	31.86	23.03
HE(TR)-O2	17	298.2	0.7370	-2.52	-31.34	-26.76	1.11	0.42	1.57	8.91	12.21	10.08
HE-O2(TR)	17	298.2	0.7180	0.06	-29.52	-24.83	3.79	3.08	4.26	11.79	15.18	12.99
HE-O2	53	323.2	0.8090	2.24	-29.42	-23.00	5.93	4.64	5.83	14.78	18.38	18.64
HE-O2	53	353.2	0.9870	-2.11	-33.91	-26.09	1.16	-0.73	0.40	10.48	14.07	16.60
HE-O2	53	383.2	1.1200	-0.51	-34.18	-24.69	2.45	-0.19	0.95	12.84	16.63	20.98
HE-O2	53	413.2	1.2450	2.12	-33.70	-22.52	4.72	1.51	2.67	16.35	20.38	26.21
HE-O2	53	443.2	1.4200	1.22	-35.43	-23.05	3.31	-0.27	0.87	15.81	19.93	26.70
HE-O2	53	473.2	1.5950	1.06	-36.58	-23.02	2.63	-1.06	0.06	16.08	20.31	27.76
HE-O2	53	498.2	1.6830	4.81	-35.07	-20.04	5.97	2.04	3.20	20.75	25.24	33.37
HE-AR	25	276.2	0.6460	-2.56	-35.76	-33.85	-9.75	-0.67	0.61	9.00	9.87	7.22
HE-AR	57	287.9	0.6970	-2.89	-36.64	-33.99	-9.97	-1.27	0.01	8.90	9.83	8.60
HE-AR(TR)	17	296.2	0.7290	-2.42	-36.78	-33.61	-9.49	-1.05	0.23	9.62	10.59	10.29
HE-AR(TR)	61	298.0	0.7250	-0.83	-35.85	-32.52	-8.01	0.53	1.84	11.44	12.44	12.33
HE-AR	61	298.0	0.7540	-4.65	-38.32	-35.12	-11.55	-3.33	-2.08	7.15	8.11	8.01
HE-AR	25	317.2	0.7968	0.65	-35.90	-31.38	-6.59	1.57	2.89	13.53	14.64	16.48
HE-AR	53	323.2	0.8090	2.44	-35.07	-30.13	-4.93	3.23	4.57	15.68	16.83	19.27
HE-AR	25	346.2	0.9244	1.11	-37.00	-30.89	-6.22	1.30	2.61	14.65	15.90	20.18
HE-AR	53	353.2	0.9780	-1.03	-38.64	-32.31	-8.23	-0.98	0.31	12.36	13.62	18.29
HE-AR	57	354.2	0.9790	-0.64	-38.44	-32.04	-7.87	-0.63	0.66	12.82	14.09	18.85
HE-AR	53	383.2	1.1220	-0.50	-39.56	-31.78	-7.93	-1.50	-0.23	13.52	14.90	21.40
HE-AR	53	413.2	1.2370	2.98	-38.61	-29.24	-5.00	0.88	2.19	18.01	19.57	27.69
HE-AR	57	418.0	1.3980	-7.02	-44.74	-36.09	-14.27	-9.07	-7.90	6.63	8.05	15.55
HE-AR	53	443.2	1.4010	2.79	-39.79	-29.22	-5.51	-0.19	1.10	18.29	19.97	29.09
HE-AR	53	473.2	1.6120	0.18	-42.27	-30.88	-8.27	-3.35	-2.10	15.75	17.49	27.08
HE-AR	53	498.2	1.7280	2.27	-41.82	-29.33	-6.70	-1.85	-0.57	18.52	20.38	30.58
HE-AR	61	500.0	1.8600	-4.39	-45.66	-33.92	-12.80	-8.27	-7.08	10.83	12.58	22.13
HE-AR	61	1000.0	6.2500	-4.29	-54.26	-32.47	-19.53	-13.04	-11.92	15.66	18.54	21.81
HE-AIR	61	1100.0	7.3800	-4.24	-55.31	-32.23	-20.69	-13.64	-12.52	16.39	19.44	20.51
HE-AIR	25	276.2	0.6242	-6.81	-33.32	-29.95	-1.26	0.09	1.14	10.09	12.72	5.21
HE-AIR	25	317.2	0.7652	-3.15	-33.06	-26.89	2.29	2.87	3.95	15.37	18.34	15.01
HE-AIR	25	346.2	0.9019	-4.23	-35.24	-27.52	0.77	0.46	1.52	14.68	17.76	16.79
HE-CO	27	295.6	0.7020	-3.95	-34.13	-29.31	-1.29	-0.28	0.75	7.37	11.24	4.29
HE-CO2	25	276.2	0.5312	-5.82	-27.47	-25.73	-2.53	-3.69	-2.39	8.69	8.14	15.28
HE-CO2	53	298.2	0.6120	-6.53	-29.37	-26.11	-2.87	-4.90	-3.61	8.37	7.94	17.81
HE-CO2	25	317.2	0.6607	-3.53	-28.23	-23.61	0.47	-2.28	-0.95	12.26	11.90	24.19
HE-CO2	53	323.2	0.6780	-2.86	-28.07	-23.03	1.23	-1.72	-0.39	13.17	12.83	25.82
HE-CO2	25	346.2	0.7646	-2.85	-29.29	-22.86	1.38	-2.20	-0.87	13.65	13.41	28.45
HE-CO2	53	353.2	0.8000	-3.84	-30.35	-23.60	0.37	-3.31	-2.00	12.63	12.42	27.85
HE-CO2	53	383.2	0.8840	0.37	-28.77	-20.07	4.78	0.29	1.64	18.13	18.04	36.22
HE-CO2	53	413.2	1.0400	-2.66	-32.21	-22.30	1.52	-3.35	-2.04	15.09	15.11	34.28
HE-CO2	53	443.2	1.1330	1.01	-30.88	-19.20	5.16	-0.25	1.10	19.93	20.06	41.13
HE-CO2	53	473.2	1.2790	0.35	-32.45	-19.57	4.22	-1.89	-0.56	19.61	19.85	41.60
HE-CO2	53	498.2	1.4140	-0.67	-33.99	-20.27	2.91	-3.52	-2.21	18.76	19.07	41.08
HE-WATER	34	298.2	0.9080	-7.69	-35.53	-28.50	-24.82	1.09	1.64	-13.66	132.88	11.14
HE-WATER	50	307.2	0.9020	-2.11	-32.14	-24.12	-19.93	6.96	7.54	-8.28	151.27	19.10
HE-WATER	50	328.5	1.0110	-1.79	-33.06	-23.72	-18.93	6.92	7.51	-7.61	162.15	22.13
HE-WATER	50	352.5	1.1210	-5.33	-36.60	-30.49	-21.19	2.76	4.15	-10.56	163.33	18.62
HE-NH3	27	296.6	0.8310	-6.05	-39.37	-32.58	-23.29	12.39	12.91	-9.73	-16.35	6.16
HE-NH3	17	297.1	0.8420	-7.00	-40.01	-33.26	-24.05	11.20	11.72	-10.63	-17.19	5.15
HE-METHANE	16	373.0	1.0050	-5.87	-31.81	-18.80	1.55	-2.10	-1.72	10.50	14.04	20.03
HE-N-HEXANE	16	417.0	0.5740	-17.50	-35.87	-28.82	-6.41	-2.22	-0.62	-1.18	19.75	5.82
HE-N-HEPTANE*	12	303.2	0.2650	-5.68	-20.09	-19.42	6.38	13.07	14.97	9.67	35.59	8.69
HE-2,4-DIMETHYLPENTANE*	12	303.2	0.2630	-4.96	-19.49	-18.80	8.02	15.22	17.15	12.11	39.87	10.75
HE-N-OCTANE	12	303.2	0.2680	-6.12	-20.04	-19.81	6.30	-3.97	-2.33	7.36	36.53	5.22
HE-2,2,4-TRIMETHYLPENT.*	12	303.2	0.2530	-7.98	-21.62	-21.39	5.33	12.68	14.61	8.41	38.34	6.15
HE-BENZENE	34	298.2	0.3840	-18.39	-30.29	-29.24	-10.43	-3.87	-2.33	-4.39	8.87	0.87
HE-BENZENE	53	423.2	0.6100	-5.20	-25.81	-16.93	5.97	9.68	11.44	13.42	29.75	28.83
HE-BENZENE	53	463.2	0.7150	-5.27	-27.52	-16.77	5.96	8.93	10.68	13.95	30.50	30.69
HE-BENZENE	53	503.2	0.8150	-3.93	-28.00	-15.38	7.38	9.83	11.59	16.14	33.15	33.97
HE-BENZENE	53	523.2	0.8610	-2.65	-27.75	-14.15	8.73	10.97	12.76	17.97	35.32	36.32
HE-NITROBENZENE*	34	298.2	0.3720	-22.65	-36.62	-36.92	-21.51	-16.07	-14.61	-17.83	-4.98	-13.28
HE-METHANOL	53	423.2	1.0320	-1.00	-30.60	-18.37	-4.66	7.35	8.57	3.21	-2.64	27.45
HE-METHANOL	53	463.2	1.2180	-1.76	-32.67	-18.17	-5.09	5.91	7.12	2.98	-2.74	28.39
HE-METHANOL	53	503.2	1.3890	-0.42	-33.15	-17.46	-3.65	6.83	8.04	4.90	-0.82	31.56
HE-METHANOL	53	523.2	1.4750	0.40	-33.26	-16.68	-2.84	7.37	8.60	6.01	0.28	33.18
HE-ETHANOL	34	298.2	0.4940	-13.75	-31.27	-28.28	-14.35	-4.18	-2.86	-4.56	-2.12	5.10
HE-ETHANOL	53	423.2	0.8210	-4.23	-30.08	-19.53	-2.51	4.27	5.71	8.22	11.49	28.30
HE-ETHANOL	53	463.2	0.9250	-0.45	-28.94	-16.12	1.57	7.73	9.22	13.11	16.67	35.40
HE-ETHANOL	53	503.2	1.0480	1.58	-28.98	-14.20	3.70	9.31	10.82	15.99	19.76	39.65
HE-ETHANOL	53	523.2	1.1730	-2.84	-32.73	-17.84	-0.82	4.22	5.65	11.20	14.87	34.12
HE-PROPANOL*	53	423.2	0.6760	-2.47	-29.01	-19.48	0.14	6.69	8.30	12.99	21.93	30.27
HE-PROPANOL*	53	463.2	0.7840	-1.50	-29.91	-18.46	1.96	7.59	9.22	15.87	29.62	33.94
HE-2-PROPANOL*	53	503.2	0.8820	1.21	-29.46	-16.01	4.72	9.95	11.61	19.65	34.00	39.11
HE-2-PROPANOL*	53	523.2	0.9880	-3.27	-33.24	-19.63	0.02	4.74	6.32	14.62	28.43	33.50
HE-BUTANOL*	53	423.2	0.5870	-1.68	-25.							

SYSTEM	REF.	TEMP. ^a	OBS. ^b	FSG ^c	ANDR ^d	HBS ^e	CH-OT ^f	OT-CH ^g	GILL ^h	ARN ⁱ	MOD-HBS ^j	SL-BD ^k	
HE-HEXANOL*	53	503.2	0.6310	1.64	-24.85	-12.73	11.97	15.33	17.28	19.24	44.40	32.27	
HE-HEXANOL*	53	523.2	0.6860	0.09	-26.71	-13.96	10.18	13.24	15.15	17.70	42.61	30.79	
N2-AR	59	293.0	0.1940	-0.27	-28.96	-27.53	-6.76	-3.35	5.01	1.87	-2.36	-7.29	
N2-CO	6	289.5	0.2110	-7.69	-31.15	-29.23	-4.76	-8.52	-1.11	-7.00	-9.17	-17.23	
N2-CO2	27	295.8	0.2120	-4.60	-29.22	-26.81	-1.49	-5.53	2.12	-3.76	-5.98	-13.78	
N2-CO2	6	289.2	0.1580	-1.50	-20.71	-19.67	-2.38	-9.04	-1.05	-0.56	-6.68	-2.98	
N2-CO2	59	293.0	0.1630	-2.31	-21.63	-20.30	-3.04	-9.65	-1.72	-1.31	-7.36	-3.31	
N2-CO2	7	298.0	0.1650	-0.59	-20.59	-18.86	-1.15	-8.01	0.06	0.53	-5.62	-1.00	
N2(TRI)-CO2	60	298.0	0.1670	-1.78	-21.54	-19.83	-2.34	-9.11	-1.13	-0.68	-6.75	-2.19	
N2-CO2(TR)	60	298.0	0.1670	-1.78	-21.54	-19.83	-2.34	-9.11	-1.13	-0.68	-6.75	-2.19	
N2-CO2(TR)	17	298.2	0.1630	0.74	-19.53	-17.76	0.18	-6.70	1.49	1.88	-4.35	0.35	
N2(TRI)-CO2	17	298.2	0.1810	-9.27	-27.53	-25.94	-9.78	-15.98	-8.60	-8.25	-13.86	-9.63	
N2-CO2	60	300.0	0.1730	-4.07	-23.49	-21.68	-4.54	-11.03	-3.23	-2.95	-8.88	-4.24	
N2-CO2	60	600.0	0.6050	-7.74	-38.12	-23.09	-5.91	-13.81	-6.24	-2.70	-7.81	5.14	
N2-CO2	60	900.0	1.2170	-6.75	-43.49	-21.32	-7.31	-14.78	-7.30	0.77	-4.03	5.39	
N2-CO2	60	1200.0	1.9760	-4.98	-46.42	-19.13	-8.51	-14.97	-7.51	4.46	-0.13	3.85	
N2-WATER	50	307.6	0.2560	8.82	-18.31	-13.57	-12.50	3.73	11.18	-5.99	9.87	14.47	
N2-WATER	50	328.6	0.3030	3.21	-23.80	-17.86	-15.96	-0.97	6.14	-10.49	8.29	10.93	
N2-WATER	50	352.2	0.3590	-1.65	-28.63	-21.57	-18.94	-4.86	1.97	-14.34	7.46	7.86	
N2-NH3	27	295.1	0.2480	1.01	-28.29	-24.89	-18.53	3.91	11.23	-11.15	-21.68	-1.73	
N2-ETHYLENE	31	291.2	0.1630	-8.46	-21.75	-19.44	-3.93	-8.30	-0.87	-2.83	-7.38	-6.30	
N2-ETHYLENE	7	298.0	0.1630	-4.68	-18.99	-16.06	0.30	-4.16	3.61	1.31	-3.40	-1.60	
N2-Ethane	7	298.0	0.1480	-0.37	-16.98	-14.16	1.36	-2.80	5.19	0.50	-0.62	-3.41	
N2-N-BUTANE	7	298.0	0.0960	3.72	-11.31	-10.20	2.02	2.56	11.88	0.81	4.80	-7.06	
N2-ISOBUTANE	7	298.0	0.0905	10.03	-5.92	-4.74	9.15	6.30	15.96	5.97	11.91	-3.21	
N2-N-HEXANE	14	288.6	0.0757	-0.50	-13.09	-13.90	-4.34	-5.22	3.71	-7.24	0.66	-17.82	
N2-2,3,3-DIMETHYLBUTANE*	14	288.7	0.0751	0.36	-12.35	-13.16	-2.83	-3.14	5.98	-4.92	3.42	-15.06	
N2-CYCLOHEXANE	14	288.6	0.0760	0.79	-6.76	-7.56	0.93	-4.47	4.51	0.14	6.24	-8.28	
N2-METHYLCYCLOPENTANE*	14	288.6	0.0760	0.79	-7.86	-8.65	0.48	-0.84	8.48	-1.08	5.81	-10.23	
N2-N-HEPTANE*	12	303.2	0.0740	2.06	-11.52	-11.56	-1.48	-2.98	6.25	-6.26	3.80	-16.75	
N2-2,4-DIMETHYLPHENATE*	12	303.1	0.0744	1.46	-12.04	-12.08	-1.04	-2.22	7.08	-5.52	5.63	-16.38	
N2-N-OCTANE	12	303.1	0.0726	-3.25	-15.79	-16.18	-6.95	-18.16	-10.31	-13.13	-1.48	-23.82	
N2-2,2,4-TRIMETHYLPHENATE*	12	303.3	0.0713	-1.38	-14.17	-14.55	-3.73	-4.69	4.45	-8.88	3.83	-20.19	
N2-N-DECANE*	14	363.6	0.0841	1.88	-16.72	-11.27	0.56	-3.12	6.28	-8.43	6.19	-17.50	
N2-2,3,3-TRIMETHYLHEPTA*	14	363.8	0.0684	25.39	4.94	9.20	24.17	19.22	30.79	12.70	30.69	1.55	
N2-N-DODECANE*	14	399.4	0.0813	12.69	-7.44	-1.64	12.50	9.92	20.67	-0.08	18.99	-9.92	
N2-BENZENE	26	311.3	0.1022	-1.62	-16.76	-13.47	-5.42	-7.12	1.56	-6.52	-3.07	-10.34	
N2-PYRIDINE*	26	317.9	0.1068	3.89	-13.62	-11.83	-5.51	-9.72	-1.28	-7.94	-1.48	-9.94	
N2-PIPERIDINE*	26	314.9	0.0953	-1.94	-13.42	-12.07	-4.32	-4.96	3.99	-4.57	1.29	-8.91	
N2-TIOPHENE*	26	302.1	0.0992	5.61	-13.99	-13.63	-6.35	-8.17	0.47	-5.43	-8.95	-8.54	
N2-TETRAHYDROTIOPHENE*	26	318.5	0.0985	0.89	-12.31	-10.76	-2.15	-4.35	4.68	-2.55	-0.88	-4.91	
O2-WATER	50	308.1	0.2820	-0.79	-20.42	-16.19	-17.35	-4.47	2.58	-13.66	-4.20	9.17	
O2-WATER	50	329.0	0.3180	-1.31	-22.12	-16.47	-16.65	-3.93	3.16	-13.78	-0.99	10.94	
O2-WATER	50	352.4	0.3520	0.55	-22.01	-14.72	-13.96	-1.40	5.87	-11.79	5.01	15.31	
O2-N-HEXANE	14	288.6	0.0753	-3.15	-11.32	-12.28	-3.48	-8.68	0.17	-10.13	-0.44	-18.21	
O2-2,3-DIMETHYLBUTANE*	14	288.6	0.0753	-3.27	-11.41	-12.38	-2.92	-7.92	1.01	-8.76	1.29	-16.89	
O2-CYCLOHEXANE	14	288.6	0.0744	-0.27	-3.08	-4.05	3.56	-6.20	2.88	-1.20	6.80	-7.00	
O2-METHYLCYCLOPENTANE*	14	287.1	0.0742	-0.91	-4.75	-5.84	2.34	-3.58	5.75	-3.10	5.65	-9.78	
O2-N-OCTANE	14	303.1	0.0705	-3.96	-12.60	-13.10	-4.26	-19.72	-11.79	-14.33	-0.51	-22.95	
O2-2,2,4-TRIMETHYLPHENATE*	14	303.0	0.0705	-4.01	-12.65	-13.15	-2.89	-8.18	0.89	-11.87	2.78	-20.84	
O2-BENZENE	26	311.3	0.1011	-3.46	-11.97	-10.79	-3.74	-9.33	-0.61	-8.48	-3.47	-9.73	
O2-PYRIDINE*	26	318.3	0.1050	2.84	-10.00	-8.25	-3.00	-11.23	-2.68	-9.10	-1.04	-8.52	
O2-PIPERIDINE*	26	315.0	0.0953	-4.94	-11.79	-10.54	-3.78	-8.34	0.53	-7.73	-0.27	-9.47	
O2-TIOPHENE*	26	302.1	0.0975	4.31	-10.58	-10.34	-4.15	-9.99	-1.28	-6.78	-8.83	-7.29	
O2-TETRAHYDROTIOPHENE*	26	318.5	0.0983	-2.10	-10.46	-9.01	-1.46	-7.74	1.23	-5.58	-2.31	-5.29	
NE-AR	49	90.0	0.0360	7.90	-6.74	-29.69	-11.79	-0.28	7.64	11.76	5.55	-56.65	
NE-AR	49	194.5	0.1530	-2.20	-28.79	-34.79	-8.20	-2.29	5.47	6.09	1.20	-23.30	
NE-AR	49	273.0	0.2710	-0.06	-33.14	-32.68	-4.55	-0.18	7.76	10.64	6.00	-6.88	
NE-AR	56	273.0	0.2760	-1.87	-34.35	-33.90	-6.27	-1.98	5.80	8.63	4.08	-8.56	
NE-AR	56	288.0	0.3000	-0.87	-34.56	-33.11	-5.25	-1.09	6.77	10.10	5.56	-5.66	
NE-AR	56	303.0	0.3270	-0.60	-35.21	-32.83	-4.99	-1.02	6.84	10.73	6.24	-3.63	
NE-AR	56	318.0	0.3570	-0.92	-36.20	-32.95	-5.33	-1.55	6.27	10.70	6.27	-2.36	
NE-AR	49	353.0	0.4140	2.57	-35.65	-30.37	-2.22	1.29	9.34	15.31	10.86	4.29	
NE-AR	49	473.0	0.6710	5.61	-38.42	-27.68	-0.91	2.55	10.69	20.83	16.60	13.98	
NE-KR	56	273.0	0.2230	-4.09	-34.33	-35.69	-6.92	-1.73	6.74	6.27	3.66	-10.34	
NE-KR	56	288.0	0.2400	-2.14	-33.89	-34.27	-4.94	0.35	8.99	8.78	6.19	-6.57	
NE-KR	56	303.0	0.2660	-3.50	-35.63	-35.09	-6.23	-1.76	6.70	7.59	5.10	-6.14	
NE-KR	56	318.0	0.2840	-1.64	-35.17	-33.74	-4.44	0.11	8.73	9.98	7.50	-2.75	
AR-KR	49	199.5	0.0720	-1.59	-22.16	-30.69	-19.97	-11.06	-2.09	-1.48	-6.87	-22.80	
AR-KR	49	273.0	0.1260	-2.64	-28.79	-30.78	-16.14	-7.78	1.52	-0.68	-5.73	-10.63	
AR-KR	56	273.0	0.1190	3.09	-24.61	-26.71	-11.21	-2.35	7.50	5.16	-0.19	-5.38	
AR-KR	56	288.0	0.1280	5.24	-24.05	-25.06	-8.68	0.33	10.45	7.71	2.30	-1.34	
AR-KR	56	303.0	0.1400	5.16	-25.07	-25.00	-8.16	0.91	11.09	7.96	2.60	0.43	
AR-KR	56	318.0	0.1530	4.72	-26.28	-25.21	-8.04	0.96	11.15	7.81	2.53	1.66	
AR-KR	49	353.0	0.1970	-2.37	-33.04	-30.05	-13.38	-5.07	4.50	1.15	-3.68	-2.21	
AR-KR	49	373.0	0.2160	-1.94	-33.66	-29.63	-12.62	-4.28	5.37	1.93	-2.87	-0.37	
AR-KR	49	473.0	0.3270	-1.84	-37.43	-29.06	-11.53	-3.33	6.43	3.49	-1.07	4.35	
AR-XE	2	194.7	0.0508	4.26	1.35	-11.48	-4.23	-4.23	4.10	5.86	7.68	3.28	-16.19
AR-XE	2	273.2	0.0962	-0.40	-11.04	-14.58	-1.35	-2.78	7.33	4.98	1.14	-4.91	
AR-XE	2	329.9	0.1366	-2.44	-16.87	-15.84	-0.45	-2.51	7.62	4.01	0.45	-0.36	
AR-XE	2	378.0	0.1759	-3.86	-20.82	-16.73	-0.30	-2.74	7.36	3.33	-0.03	1.91	
AR-CO	27	295.7	0.1880	2.66	-24.34	-22.63	-0.42	1.38	10.16	4.67	0.81	-4.07	
AR-CO2	25	276.2	0.1326	1.16	-18.08	-18.69	-7.82	-8.35	0.26	3.12	-4.63	0.93	
AR-CO2	25	317.2	0.1652	3.45	-19.07	-16.51	-3.69	-4.86	4.08	6.34	-1.48	8.55	
AR-NH3	27	295.1	0.2320	5.43	-25.73	-23.33	-22.16	7.19	15.25	-6.06	-18.65	6.90	
AR-N-HEXANE	14	288.6	0.0663	2.40	-10.83	-12.03	-9.28	-5.67	3.86	-4.33	4.35	-14.59	
AR-2,3-DIMETHYLBUTANE*													

SYSTEM	REF.	TEMP. ^a	OBS. ^b	FSG ^c	ANDR ^d	HBS ^e	CH-OT ^f	OT-CH ^g	GILL ^h	ARN ⁱ	MOD-HBS ^j	SL-BD ^k
CO ₂ -N ₂ O	1	273.2	0.0989	-0.15	-2.20	-3.45	-1.54	-7.21	1.64	8.49	-2.04	13.78
CO ₂ -N ₂ O	6	287.3	0.1070	-0.79	-2.51	-2.40	0.53	-5.40	3.62	9.84	-0.76	17.15
CO ₂ -N ₂ O	62	298.0	0.1170	-1.74	-5.82	-4.74	-1.22	-7.33	1.51	7.32	-2.98	15.77
CO ₂ -N ₂ O	1	312.8	0.1280	-2.23	-7.42	-5.08	-0.73	-7.06	1.80	7.10	-3.13	17.15
CO ₂ -N ₂ O	1	362.8	0.1683	-3.61	-12.05	-6.00	0.53	-7.42	1.40	6.53	-3.46	20.69
CO ₂ -WATER	50	307.5	0.2020	10.08	-7.13	-3.49	-16.34	-5.66	1.67	-4.34	-13.69	28.92
CO ₂ -WATER	50	328.6	0.2110	18.36	-1.79	3.98	-8.36	3.10	11.11	3.27	-3.53	41.66
CO ₂ -WATER	50	352.4	0.2450	15.21	-6.06	1.42	-9.16	1.45	0.33	0.94	-2.19	40.72
CO ₂ -PROPANE	62	298.0	0.0863	6.96	-1.28	-0.15	-0.62	-8.16	0.60	3.52	0.74	6.49
CO ₂ -ETHYLENEOXIDE*	62	298.0	0.0918	15.09	17.53	18.87	11.02	-4.72	4.36	11.10	0.45	22.70
N ₂ O-PROPANE	62	298.0	0.0860	-1.35	-2.58	-1.46	-5.06	-8.20	0.55	2.76	-0.36	5.77
N ₂ O-ETHYLENEOXIDE*	62	298.0	0.0914	6.91	15.84	17.17	5.89	-4.93	4.13	10.31	-0.56	21.88
NH ₃ -SF ₆	27	296.6	0.1090	15.15	-2.05	-3.58	-8.98	1.35	9.86	5.88	-1.96	18.38
METHANE-WATER	50	307.7	0.2920	-3.00	-16.99	-10.32	-21.62	-8.95	-3.41	-15.25	-10.76	11.52
METHANE-WATER	50	328.8	0.3310	-3.90	-19.11	-10.98	-21.01	-8.62	-3.06	-15.70	-8.10	12.90
METHANE-WATER	50	352.3	0.3560	0.83	-16.59	-6.41	-15.75	-3.27	2.62	-11.19	0.39	20.86
ETHYLENE-WATER	50	307.8	0.2040	0.23	-10.05	-4.81	-19.05	-7.21	-0.55	-8.68	-13.78	20.47
ETHYLENE-WATER	50	328.5	0.2330	-1.65	-13.17	-6.42	-19.12	-7.56	-0.92	-10.05	-12.12	20.74
ETHYLENE-WATER	50	352.3	0.2470	4.85	-9.03	-0.02	-12.17	-0.02	7.16	-3.70	-2.41	31.37
FREON12*-WATER	34	298.2	0.1050	-0.53	13.26	12.33	-7.15	4.13	12.97	2.07	-4.53	25.57
FREON12*-BENZENE	34	298.2	0.0385	-7.76	7.91	5.64	-14.17	-14.13	-4.39	-5.13	-4.53	-11.06
FREON12*-ETHANOL	34	298.2	0.0475	6.62	22.57	20.73	-2.39	1.23	11.95	10.56	5.00	11.01
AIR-CL ₂	3	293.0	0.1240	0.08	-16.11	-16.04	-1.04	-6.50	2.23	1.80	-3.07	0.39
AIR-BK ₂	3	293.0	0.0910	0.03	1.20	-1.23	9.84	4.50	14.78	13.54	12.89	13.33
AIR-CO ₂	25	276.2	0.1420	-3.48	-17.17	-17.21	0.88	-7.32	0.88	1.72	-4.97	-1.51
AIR-CO ₂	3	293.0	0.1650	-7.89	-22.12	-20.85	-3.06	-10.93	-3.06	-2.59	-8.92	-3.84
AIR-CO ₂	25	317.2	0.1772	-1.45	-18.31	-15.12	4.56	-4.30	4.17	4.72	-1.99	5.76
AIR-SO ₂	3	293.0	0.1220	0.03	-10.88	-10.52	-0.11	-0.35	8.86	5.32	-0.82	4.86
AIR-WATER	34	298.2	0.2600	-3.25	-22.36	-18.66	-17.46	-3.61	3.36	-12.10	-0.64	7.00
AIR-WATER	18	299.1	0.2580	-1.98	-21.40	-17.59	-16.33	-2.17	4.90	-10.93	0.84	8.51
AIR-WATER	18	312.6	0.2770	-1.37	-21.78	-16.97	-15.07	-1.03	6.13	-10.14	4.11	10.87
AIR-WATER	18	333.2	0.3050	0.16	-21.83	-15.52	-12.73	1.30	8.63	-8.40	9.74	14.90
AIR-NH ₃	27	295.1	0.2470	-3.18	-27.24	-23.89	-16.79	4.62	12.04	-10.44	-21.42	-0.09
AIR-METHANE	13	289.0	0.2190	-8.86	-21.65	-18.41	0.32	-6.19	0.31	-2.67	-6.15	-5.26
AIR-METHANE	13	294.6	0.2240	-7.85	-21.16	-17.46	1.61	-4.93	1.66	-1.48	-4.98	-3.52
AIR-BENZENE	34	298.2	0.0962	-6.96	-15.01	-14.80	-6.59	-10.11	-1.65	-8.70	-5.49	-12.95
AIR-BENZENE	28	308.0	0.1021	-7.23	-15.95	-14.96	-6.32	-9.76	-1.27	-8.80	-5.54	-12.21
AIR-TOLUENE	18	299.1	0.0860	-5.95	-15.09	-15.25	-7.21	-11.43	-2.98	-9.95	-3.79	-15.83
AIR-TOLUENE	18	312.6	0.0920	-5.02	-15.20	-14.30	-5.53	-9.85	-1.26	-8.82	-2.52	-13.69
AIR-TOLUENE	18	333.2	0.1040	-6.06	-17.45	-15.07	-5.54	-10.15	-1.58	-9.47	-3.13	-12.88
AIR-CHLOROBENZENE*	18	299.1	0.0740	8.13	-0.81	-1.61	6.74	2.00	11.85	3.42	8.51	-2.55
AIR-CHLOROBENZENE*	18	312.6	0.0790	9.42	-0.73	-0.31	8.94	3.92	13.96	4.93	10.16	0.13
AIR-CHLOROBENZENE*	18	333.2	0.0900	7.39	-4.11	-1.96	8.15	3.01	12.96	3.38	8.63	0.30
AIR-ANILINE*	18	299.1	0.0740	14.94	1.32	1.10	6.06	6.88	17.08	10.34	11.22	7.37
AIR-ANILINE*	18	312.6	0.0790	16.32	1.41	2.44	8.31	9.03	19.44	11.95	12.91	10.33
AIR-ANILINE*	18	333.2	0.0900	14.17	-2.05	0.74	7.63	8.19	18.51	10.30	11.34	10.51
AIR-NITROBENZENE*	34	298.2	0.0855	-6.68	-17.91	-18.87	-14.96	-18.84	-10.95	-17.42	-13.84	-21.88
AIR-DIPHENYL*	18	490.0	0.1600	-7.10	-23.62	-13.82	-2.79	-6.28	2.92	-11.75	0.48	-12.94
AIR-ETHANOL	34	298.2	0.1350	-8.58	-20.50	-18.93	-13.95	-13.16	-5.43	-11.64	-16.46	-10.94
AIR-2-PROPANOL*	18	299.1	0.0990	4.55	-7.96	-6.86	1.78	-0.89	8.22	2.14	3.87	-1.17
AIR-2-PROPANOL*	18	312.6	0.1070	4.51	-9.01	-6.78	2.52	-0.26	8.91	2.37	4.16	0.31
AIR-2-PROPANOL*	18	333.2	0.1210	3.33	-11.46	-7.65	2.44	-0.47	8.68	1.61	3.47	1.22
AIR-BUTANOL*	18	299.1	0.0870	3.89	-7.77	-7.30	-0.40	-2.22	6.94	-1.02	6.28	-6.12
AIR-BUTANOL*	18	312.6	0.0920	6.13	-6.81	-5.17	2.61	0.45	9.67	1.39	8.93	-2.62
AIR-BUTANOL*	18	333.2	0.1040	4.98	-9.28	-6.02	2.65	0.24	9.64	0.68	8.25	-1.70
AIR-2-BUTANOL*	18	299.1	0.0890	1.56	-9.84	-9.38	-1.62	-3.86	5.15	-2.67	6.07	-8.23
AIR-2-BUTANOL*	18	312.6	0.0960	1.71	-10.69	-9.12	-0.67	-3.08	6.01	-2.26	6.58	-6.67
AIR-2-BUTANOL*	18	333.2	0.1080	1.09	-12.64	-9.50	-0.19	-2.72	6.40	-2.48	6.42	-5.34
AIR-2-PENTANOL*	18	299.1	0.0710	14.27	2.07	2.02	11.18	9.12	19.49	8.82	18.22	0.12
AIR-2-PENTANOL*	18	312.6	0.0760	15.33	1.88	3.10	13.12	11.04	21.59	10.11	19.70	2.61
AIR-2-PENTANOL*	18	333.2	0.0860	13.96	-0.92	2.07	13.01	10.70	21.22	9.22	18.83	3.47
AIR-ETHYLACETATE	18	299.1	0.0870	0.85	-11.54	-11.58	-1.95	-2.95	6.28	-3.60	-1.38	-10.22
AIR-ETHYLACETATE	18	312.6	0.0940	0.84	-12.53	-11.48	-1.20	-2.17	7.13	-3.36	-1.08	-8.85
AIR-ETHYLACETATE	18	333.2	0.1060	-0.01	-14.64	-12.06	-1.02	-1.92	7.40	-3.81	-1.45	-7.76
AIR-HCN*	30	273.0	0.1730	-9.96	-21.22	-20.35	-15.77	-31.65	-76.11	-26.84	-37.15	-26.71
AIR-CYANODICHLORIDE*	30	273.0	0.1110	-2.75	-12.36	-13.62	-5.05	-16.27	-8.56	-11.68	-13.69	-16.29
AIR-PHOSGENE*	30	273.0	0.0950	-7.94	-15.06	-17.54	-6.88	-12.68	-4.31	-8.65	-7.88	-15.58
AIR-CHLOROPICRICIN*	30	298.0	0.0880	-6.32	-17.59	-19.26	-10.74	-15.86	-7.57	-15.19	-9.00	-21.65
AVE. ERROR (PER CENT)				4.32	21.11	16.57	10.67	6.38	6.76	8.86	14.02	13.89
STANDARD DEVIATION (PER CENT)				6.71	24.34	19.24	15.41	8.72	8.91	10.95	23.73	17.67

^a Temperature (°K)

^b OBS = Experimentally observed diffusion coefficient reduced to 1 atm. pressure (cm.²/sec.)

^c FSG = Value obtained in this work

^d ANDR = Value obtained from Andrussow (4)

^e HBS = Value obtained from Hirschfelder-Bird-Spotz (20-22)

^f CH-OT = Value obtained from Chen-Othmer (77)

^g OT-CH = Value obtained from Othmer-Chen (41)

^h GILL = Value obtained from Gilliland (78)

ⁱ ARN = Value obtained from Arnold (5)

^j MOD-HBS = Values obtained from the Wilke-Lee modification of HBS (64)

^k SL-BD = Value obtained from Slattery-Bird (54)

* Indicates that, in the HBS and MOD-HBS calculations, force constants for the starred components were estimated from critical properties.

Arnold method is seen to perform substantially better than the other methods based mainly on the Le Bas parameters. The well known HBS method is seen to be quite reliable with an average error of only 6.4%. Wilke and Lee's modification of the HBS method is seen to improve results in some cases, but the average overall error is increased by its use.

The Slattery-Bird method is seen to give good agreement on N₂ systems, but in the case of He systems and to a somewhat lesser extent for H₂ systems, its use can lead to rather large errors. This is expected since the authors state that their correlation is not applicable to He and H₂ systems. Thus the error for systems with these gases should not be charged against this method.

The Chen-Othmer correlation gives good results close to room temperature, but for some systems the 1.81 temperature dependence of this method appears too high. The Othmer-Chen reference substance method shows poorer agreement than expected, with an average error of 13.9%. The present diffusion volume correlation with an average error of 4.3% shows the best agreement between calculated and observed values in each of the categories of Table II. Furthermore, if the maximum permissible per cent error is taken arbitrarily to be 10%, the correlation developed here has far fewer points in error greater than this amount than any of the other methods.

Conclusion

From the above comparison it is seen that the diffusion volume correlation gives the best fit to the data used in this report. If force constants from viscosity data are available for use with the HBS method, comparable results are obtained. Average error using estimated force constants, starred points in Table III, was 8.9%; excluding starred points 5.4%. It is apparent that the HBS method rests on firm theoretical grounds while the present method can be no more reliable than the diffusion data used in its development. Any systematic errors in the data would be reflected in the atomic diffusion volumes and would lead to error through their use.

The present method has the advantage of being able to overcome the general lack of accuracy associated with other category one methods, and it is still simple to use. The additional advantage of wide applicability is a major one. It should be noted that supplementary data needed for category two methods, although limited to common substances, can be estimated using procedures described in the literature, but this adds considerably to the labor of calculation and adds an additional element of uncertainty. The diffusion volume correlation should prove useful in such cases.

Use of the diffusion volume correlation or alternatively the HBS method according to the preceding recommendations should be a valuable aid in the estimation of binary gas-phase diffusion coefficients in the absence of experimental data. Some caution is still necessary when estimating D_{AB} for systems not included in this study since in extreme cases the error of estima-

tion from either method may apparently exceed the average by a wide margin. In general, satisfactory results will be obtained since the average error of both methods is probably close to the average experimental error.

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