

Review Article

Solubility Parameters of Permanent Gases

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The solubility parameters, $\delta_H(T_b)$, of nonreactive permanent gases at their boiling points T_b (<290 K) are calculated from individually discussed values of their molar enthalpies of vaporization and densities obtained from the literature. These values are tabulated and where available the coefficients of the temperature dependence expression $\delta_H(T)$ are also tabulated. The trends noted in the $\delta_H(T_b)$ values are dealt with and the values are compared with those reported in the literature and derived from the solubilities of the gases in various solvents. The $\delta_H(T_b)$ values are shown to correlate linearly with the depths of the potential wells (attractive interaction energies, ϵ/k_B) for binary collisions of the gaseous molecules and with the surface tensions, $\sigma(T_b)$, of the liquefied gases.

1. Introduction

The solubility of gases in liquid solvents is an important issue in many fields of chemistry and chemical engineering, from processing to environmental elimination. In this review the solubility of permanent, nonreactive gases is dealt with, in terms of their solubility parameters at the normal boiling points of the liquefied gases and their temperature dependence. Permanent gases are those substances that are gaseous at ambient conditions, that is, at atmospheric pressure and ≤ 290 K. Nonreactive gases include those that dissolve in their molecular (atomic for noble gases) form in the solvents without causing chemical changes in them. This limit excludes gases like F_2 , Cl_2 , the hydrogen halides, NO_2 , and a few others. Still, this review is not exhaustive but attempts to include practically all the inorganic gases and most of the organic ones up to butane. The normal boiling points, T_b , of the liquefied gases are selected because the required data mainly pertain to these conditions (at which the vapor pressures of the saturated liquefied gases reach 101.325 kPa or one atm). T_b are also considered to be “corresponding states” as is indicated by the Trouton constant (the molar entropy of vaporization at T_b) being the same, $\Delta_v S(T_b) = 10.5R$, for ordinary (nonassociating) liquids.

1.1. Gas Solubility from Regular Solution Theory. The gases dealt with here are generally non- or only mildly polar and

their solubilities can be described by means of the regular solution theory of Hildebrand [1]. This states that the mole fraction solubility x_G of the solute gas (subscript G) in the liquid solvent (subscript S) is as follows:

$$\ln x_G = \ln x_G^{\text{id}} - \left(\frac{V_G}{RT} \right) (\delta_{HG} - \delta_{HS})^2, \quad (1)$$

where V_G is the molar volume and the two δ_H 's are the total (Hildebrand) solubility parameters. The ideal solubility at the temperature T , x_G^{id} , is given by

$$\ln x_G^{\text{id}} = \left(\frac{\Delta_v H_G(T_b)}{R} \right) (T_b^{-1} - T^{-1}), \quad (2)$$

where $\Delta_v H_G(T_b)$ is the molar enthalpy of vaporization of the liquefied solute gas at its normal boiling point T_b . In the cases of polar solutes or solvents or those prone to hydrogen bonding the partial (Hansen) solubility parameters [2] of such solvents should be used instead for the prediction of the gas solubilities, but this needs not concern much the present review. The solubility parameters of liquid solvents, δ_{HS} , are available in compilations for molecular [3, 4] and ionic [5, 6] solvents.

The solubility of a gas in a liquid is often expressed as the Henry constant, $H_{G(S)}$, which is related to the mole fraction solubility in the solvent, $x_{G(S)}$, as follows:

$$H_{G(S)} = \frac{p_G}{x_{G(S)}}, \quad (3)$$

where p_G is the partial pressure of the gas that is at equilibrium with its saturated solution. Hence, the larger the measured Henry constant, the smaller the actual (mole fraction) solubility. The solubility of a permanent gas is generally not needed at its normal boiling point, but $\delta_{HG}(T_b)$ is a reference value from which the temperature dependence of δ_{HG} can be used to obtain the value at the desired temperature. Such temperature dependence data, unfortunately, are available for only a minority of gaseous solutes.

1.2. Hildebrand Solubility Parameters. The values of the total (Hildebrand) solubility parameter of the gases dealt with here, δ_{HG} , are obtained as the square roots of the cohesive energy densities, ced_G . The latter are obtained from the molar enthalpies of vaporization and the molar volumes, assuming the liquefied gas vaporizes without association or dissociation to an ideal gas at T_b , that is, at 101.325 kPa, as follows:

$$ced_G = \delta_{HG}^2 = \frac{(\Delta_v H_G(T_b) - RT_b)}{V_G(T_b)}. \quad (4)$$

2. The Required Data

In the following the subscript G is dropped, because only the solute gases are being dealt with. The required data for obtaining the solubility parameters δ_H are the normal boiling points of the liquefied gases, T_b , their molar enthalpies of vaporization $\Delta_v H(T_b)$, and their molar volumes $V(T_b)$ at the boiling point. The molar volumes V are obtained from the ratios of the molar masses M and the densities ρ : $V = M/\rho$. The molar volume is also the reciprocal of the concentration c : $V/\text{cm}^3 \text{ mol}^{-1} = 1000/(c/\text{mol dm}^{-3})$. The molar masses and boiling points are taken from the Handbook [7]. The other quantities are obtained from the literature, from primary sources as noted below when readily available or else from secondary sources (compilations) such as [8–11].

Following are details of the data used and the results of the application of (2), yielding $\delta_H(T_b)/\text{MPa}^{1/2}$ values.

2.1. Specific Data for Each Gas

2.1.1. Helium. The earliest report of the solubility parameter of helium is that of Clever et al. [20], derived from its solubility in hydrocarbons and fluorocarbons, and is tabulated at the normal boiling point as $0.5 \text{ cal}^{1/2} \text{ cm}^{-3/2}$ (i.e., $1.02 \text{ MPa}^{1/2}$). However the text above the table states that $0.6 \text{ cal}^{1/2} \text{ cm}^{-3/2}$ (i.e., $1.23 \text{ MPa}^{1/2}$) is “more compatible with the solubility parameter at the gas b.p.”. The subsequent report by Yosim and Owens [21] evaluated the molar enthalpy of vaporization, using the scaled particle theory, but reported also its experimental value and the density at the boiling point [22], from which the value $1.20 \text{ MPa}^{1/2}$ is derivable. The most recent report is by Donnelly and Barenghi [23], who presented density and vapor pressure data at 0.05 K intervals around the boiling point that interpolate to $T_b = 4.22 \text{ K}$ and

$\rho(T_b) = 0.1250 \text{ g cm}^{-3}$. They also presented four reports for $\Delta_v H$ at 4.207 K that average at $83.04 \pm 0.37 \text{ J mol}^{-1}$, from which the solubility parameter $\delta_H(T_b) = 1.22 \pm 0.01 \text{ MPa}^{1/2}$ is derived and represents the selected value.

2.1.2. Neon. The $\delta_H(T_b)$ value tabulated by Clever et al. [20], obtained as described for He, is $4.9 \text{ cal}^{1/2} \text{ cm}^{-3/2}$ (i.e., $10.02 \text{ MPa}^{1/2}$). The value $\delta_H(T_b) = 9.49 \text{ MPa}^{1/2}$ is derived from the [22] data reported by Yosim and Owens [21]. Linford and Thornhill [24] reported the energy of vaporization as $\Delta_v E(T_b)$ (presumably $\Delta_v H - RT_b$) = $0.37 \text{ kcal mol}^{-1}$ and with the density from Gladun [25], $0.06093 \text{ mol cm}^{-3}$, the value $\delta_H(T_b) = 8.98 \text{ MPa}^{1/2}$ is derived. Leonhard and Deiters [26] reported the densities and the molar enthalpy of the gas and liquid at 5 K intervals between 25 and 40 K. The difference in the latter yields $\Delta_v H$ values, so the expression shown in Table 3 results, from which follows the value $\delta_H(T_b) = 10.01 \text{ MPa}^{1/2}$. The value $\delta_H(T_b) = 10.01 \text{ MPa}^{1/2}$ from [26], agreeing with that of [20], is adopted as the selected value for Ne.

2.1.3. Argon. The $\delta_H(T_b)$ value tabulated by Clever et al. [20], obtained as described for He, is $7.0 \text{ cal}^{1/2} \text{ cm}^{-3/2}$ (i.e., $14.32 \text{ MPa}^{1/2}$). The value $\delta_H(T_b) = 14.19 \text{ MPa}^{1/2}$ is derived from the data of [22] reported by Yosim and Owens [21]. Much lower values were reported by Prausnitz and Shair [27] at an unspecified temperature, $5.33 (\text{cal/cm}^3)^{1/2}$ (i.e., $10.90 \text{ MPa}^{1/2}$), that was quoted by LaPack et al. [28]. Chen et al. [29] presented the molar volumes and the molar enthalpies of vaporization or Ar at 17 temperatures between the triple and boiling points, from which the expression for the solubility parameter shown in Table 3 results and $\delta_H(T_b) = 14.07 \text{ MPa}^{1/2}$. Linford and Thornhill [24] reported the energy of vaporization as $\Delta_v E(T_b) = 1.385 \text{ kcal mol}^{-1}$ and with the molar volume from Terry et al. [30], $V(T_b) = 28.713 \text{ cm}^3 \text{ mol}^{-1}$, the value $\delta_H(T_b) = 14.21 \text{ MPa}^{1/2}$ is derived. The average of the four agreeing values, $14.21 \pm 0.10 \text{ MPa}^{1/2}$, is adopted as the representative value for $\delta_H(T_b)$.

2.1.4. Krypton. The $\delta_H(T_b)$ value tabulated by Clever et al. [20], obtained as described for He, is $7.5 \text{ cal}^{1/2} \text{ cm}^{-3/2}$ (i.e., $15.34 \text{ MPa}^{1/2}$). The value $\delta_H(T_b) = 15.21 \text{ MPa}^{1/2}$ is derived from the data of [22] reported by Yosim and Owens [21]. Much lower values were reported by Prausnitz and Shair [27] at an unspecified temperature, $6.4 (\text{cal/cm}^3)^{1/2}$ (i.e., $13.09 \text{ MPa}^{1/2}$). Chen et al. [29] presented the molar volumes and the molar enthalpies of vaporization of Kr at 19 temperatures between the triple and boiling points, from which the expression for the solubility parameter shown in Table 3 results and $\delta_H(T_b) = 15.18 \text{ MPa}^{1/2}$. Linford and Thornhill [24] reported the energy of vaporization as $\Delta_v E(T_b) = 2.00 \text{ kcal mol}^{-1}$ and with the molar volume from Terry et al. [30], $V(T_b) = 34.731 \text{ cm}^3 \text{ mol}^{-1}$, the value $\delta_H(T_b) = 14.57 \text{ MPa}^{1/2}$ is derived. The average of the three agreeing values, $15.24 \pm 0.09 \text{ MPa}^{1/2}$, is adopted as the representative value for $\delta_H(T_b)$.

2.1.5. Xenon. The $\delta_H(T_b)$ value tabulated by Clever et al. [20], obtained as described for He, is $8.0 \text{ cal}^{1/2} \text{ cm}^{-3/2}$ (i.e., $16.36 \text{ MPa}^{1/2}$). The value $\delta_H(T_b) = 16.19 \text{ MPa}^{1/2}$ is derived from the data of [22] reported by Yosim and Owens [21]. Chen et al. [29] presented the molar volumes and the molar enthalpies of vaporization of Xe at 17 temperatures between the triple and boiling points, from which the expression for the solubility parameter shown in Table 3 results and $\delta_H(T_b) = 15.79 \text{ MPa}^{1/2}$. Linford and Thornhill [24] reported the energy of vaporization as $\Delta_v E(T_b) = 2.69 \text{ kcal mol}^{-1}$ and with the molar volume from Terry et al. [30], $V(T_b) = 44.68 \text{ cm}^3 \text{ mol}^{-1}$ (interpolated), the value $\delta_H(T_b) = 14.87 \text{ MPa}^{1/2}$ is derived. The average of the three largest values, $16.1 \pm 0.3 \text{ MPa}^{1/2}$, is adopted as the representative value for $\delta_H(T_b)$.

2.1.6. Radon. Prausnitz and Shair [27] reported a low value (compared with the other noble gases) at an unspecified temperature, $6.83 (\text{cal/cm}^3)^{1/2}$ (i.e., $13.97 \text{ MPa}^{1/2}$). A value better compatible with the other noble gases was reported by Lewis et al. [31], $8.42 \pm 0.11 \text{ cal}^{1/2} \text{ cm}^{-3/2}$ (i.e., $17.22 \pm 0.23 \text{ MPa}^{1/2}$) at an unspecified temperature, derived from the solubility of Rn in fluorocarbon solvents. The molar enthalpy of vaporization $\Delta_v H = 16.36 \text{ kJ mol}^{-1}$ and the liquid density $\rho = 4329 \text{ kg m}^{-3}$ reported recently by Mick et al. [32], at the boiling point of ^{222}Rn , 210.5 K, were obtained from Monte Carlo simulations, leading to $\delta_H(T_b) = 16.88 \text{ MPa}^{1/2}$. Mick et al. quoted experimental values obtained more than 100 years ago for the enthalpy of vaporization, $\Delta_v H/\text{kJ mol}^{-1} = 16.59$ and 16.78 , but not highly accurate liquid densities. With the density from the simulation, these two enthalpy values yield $\delta_H(T_b)/\text{kJ mol}^{-1} = 17.01$ and $17.12 \text{ MPa}^{1/2}$. The average of the four agreeing values, 17.06 ± 0.15 , is selected here as representative.

2.1.7. Hydrogen. Yosim and Owens [21] quoted $\Delta_v H$ data from Stull and Sinke [33] leading to $\delta_H(T_b) = 5.08 \text{ MPa}^{1/2}$. Linford and Thornhill [24] reported the energy of vaporization as $\Delta_v E(T_b) = 0.175 \text{ kcal mol}^{-1}$ and with the molar volume from Van Isterbeek et al. [34] interpolated to T_b , $V(T_b) = 28.375 \text{ cm}^3 \text{ mol}^{-1}$, the value $\delta_H(T_b) = 5.08 \text{ MPa}^{1/2}$ is derived. The reference data by Leachman et al. [35] showed liquid density and gas and liquid molar enthalpy values at temperatures between 14 and 21 K that yield the expression shown in Table 3 and $\delta_H(T_b) = 5.08 \text{ MPa}^{1/2}$. Sistla et al. [36] quote Hansen [2] and report $\delta_d = 5.1 \text{ MPa}^{1/2}$ at 298 K and 1 atm for the dispersion partial solubility parameter. The well agreeing value from three authors, $\delta_H(T_b) = 5.08 \text{ MPa}^{1/2}$, is the selected value.

2.1.8. Nitrogen. Gjaldbaek and Hildebrand [37] assigned to nitrogen the value $\delta_H = 5.3 \text{ cal}^{1/2} \text{ cm}^{-3/2}$ ($10.84 \text{ MPa}^{1/2}$) in order to fit its solubility in several solvents at 298 K. Yosim and Owens [21] quoted $\Delta_v H$ data from Rossini et al. [9] leading to $\delta_H(T_b) = 11.96 \text{ MPa}^{1/2}$. Linford and Thornhill [24] reported the energy of vaporization as $\Delta_v E(T_b) = 1.18 \text{ kcal mol}^{-1}$ and with the molar volume from Terry et al. [30] $34.91 \text{ cm}^3 \text{ mol}^{-1}$

the value $\delta_H(T_b) = 11.89 \text{ MPa}^{1/2}$ is derived. Jordan et al. [38] reported the molar enthalpy of vaporization from the Handbook [7], 5569 J mol^{-1} , and the density $\rho = 0.8801 \text{ g cm}^{-3}$ at $T_b = 77.35 \text{ K}$, yielding $\delta_H(T_b) = 11.92$. The experimental latent heat of vaporization (at an unspecified temperature, presumably T_b) of 201.2 J g^{-1} yields with $\rho = 0.8801 \text{ g cm}^{-3}$ the value $\delta_H(T_b) = 12.02$. Sistla et al. [36] quote Hansen [2] and report $\delta_d = 11.9 \text{ MPa}^{1/2}$ at 298 K and 1 atm for the dispersion partial solubility parameter. The mean value from the five mutually agreeing reports, $\delta_H(T_b) = 11.95$, is selected here.

2.1.9. Oxygen. Suyama and Oishi [39] quoted earlier-published molar enthalpies of vaporization at the boiling point that agree with their own value, $6822.7 \text{ J mol}^{-1}$. This value is somewhat larger than that used by Yosim and Owens [21] from Kelley and King [40], 6812 J mol^{-1} . These two values with the molar volume interpolated in Terry et al. [30] data, $28.135 \text{ cm}^3 \text{ mol}^{-1}$, yield the solubility parameters $\delta_H(T_b) \text{ MPa}^{1/2} = 14.69$ and 14.68 , respectively. A much lower value, at an unspecified temperature, was reported by Prausnitz and Shair [27], $\delta_H = 4.0 (\text{cal/cc})^{1/2}$, $8.18 \text{ MPa}^{1/2}$, quoted by LaPack et al. [28]. A value was also derived from the molar energy of vaporization at the boiling point reported by Linford and Thornhill [24], $1.45 \text{ kcal mol}^{-1}$, yielding $\delta_H(T_b) \text{ MPa}^{1/2} = 14.69$. Molecular dynamics simulations by Zasetzky and Svishchev [41] yielded $\Delta_v H/\text{J mol}^{-1} = 6934$, 6232 , and 5083 at $T/\text{K} = 84$, 100 , and 120 , respectively. These yield with the density data the following solubility parameter values: $\delta_H(T) \text{ MPa}^{1/2} = 15.11$, 13.56 , and 11.13 at these three temperatures, interpolating to $\delta_H(T_b) \text{ MPa}^{1/2} = 14.55$ and yielding the data shown in Table 3. Sistla et al. [36] quote Hansen [2] and report $\delta_d = 11.9 \text{ MPa}^{1/2}$ at 298 K and 1 atm for the dispersion partial solubility parameter. From the four agreeing values at the boiling point, the average $\delta_H(T) \text{ MPa}^{1/2} = 14.64 \pm 0.07$ is taken as selected.

2.1.10. Boron Trifluoride. No data regarding the molar enthalpy of vaporization of liquid BF_3 were found, except for the entry in the Handbook [7] that was not traced to a definite reference, of $\Delta_v H/\text{J mol}^{-1} = 19330$. The boiling point was given there as -101°C , that is, 172.2 K . The density of liquid BF_3 was obtained from Fischer and Weidemann [42] as $\rho(t/^\circ\text{C})/\text{g cm}^{-3} = 1.68[1 - 0.0023(t + 128)]$, that is, 1.5757 g cm^{-3} at T_b . These data yield $\delta_H(T_b) \text{ MPa}^{1/2} = 20.39$, but there is no corroboration of this value from any other source.

2.1.11. Boron Trichloride. The vapor pressure of liquefied BCl_3 was reported by Fetisov et al. [43] as $\log p = 7.4311 - 1298.0/T$, from which by the Clausius-Clapeyron expression $\Delta_v H = RT^2(d \ln p/dT) = 24840 \text{ J mol}^{-1}$, at $T_b = 12.65^\circ\text{C}$ [7] = 285.8 K ($T_b = 12.1^\circ\text{C}$ was given in [43] and $\Delta_v H(T_b) = 23.77 \text{ kJ mol}^{-1}$ was given in [7]). The density of liquefied BCl_3 was reported by Ward [44] from -44 to $+5^\circ\text{C}$, being linear with the temperature and a brief extrapolation to $T_b = 12.65^\circ\text{C}$ yields $\rho(t/^\circ\text{C})/\text{g cm}^{-3} = 1.3472$ (extrapolation to 11.0°C yields $\rho/\text{g cm}^{-3} = 1.3493$, in agreement with the value reported

by Briscoe et al. [45]). These data yield $\delta_H(T_b)\text{MPa}^{1/2} = 16.07$.

2.1.12. Carbon Monoxide. Prausnitz and Shair [27] reported $\delta_H = 3.13\text{ (cal/cc)}^{1/2}$, that is, $6.40\text{ MPa}^{1/2}$, a very low value compared to other reports. Yosim and Owens [21] used the $\Delta_v H$ data of Kelley and King [40], from which the value $\delta_H(T_b)\text{MPa}^{1/2} = 12.37$ is derived. Goodwin [46] presented enthalpy of vaporization and density data from the melting to the boiling points that yield the expression shown in Table 3 and $\delta_H(T_b)\text{MPa}^{1/2} = 12.29$. Linford and Thornhill [24] reported $1.28\text{ kcal mol}^{-1}$ for the molar energy of vaporization at the boiling point, yielding with the molar volume data of Terry et al. [30], interpolated to T_b , $V = 35.53\text{ cm}^3\text{ mol}^{-1}$ and the value $\delta_H(T_b)\text{MPa}^{1/2} = 12.27$. Barreiros et al. [47] reported the molar enthalpy of vaporization and the molar volume at 80 to 125 K, and at the boiling point 5991 kJ mol^{-1} and $35.373\text{ cm}^3\text{ mol}^{-1}$, from which $\delta_H(T_b)\text{MPa}^{1/2} = 12.26$ is derived. The temperature dependence at temperatures above those in Goodwin's paper [46] is shown in Table 3. Prausnitz and Shair [27] quote Hansen [2] and report $\delta_d = 11.5\text{ MPa}^{1/2}$ at 298 K and 1 atm for the dispersion partial solubility parameter, but the total, Hildebrand solubility parameter included a contribution from the polar interactions of these gas molecules, adding up to $\delta_H(298\text{ K})\text{MPa}^{1/2} = 12.50$. The average of the four agreeing values, $\delta_H(T_b)\text{MPa}^{1/2} = 12.30 \pm 0.05$ is taken as selected.

2.1.13. Carbon Dioxide. Carbon dioxide sublimes from the solid to the gas without passing at ambient pressures through a liquid phase. Prausnitz and Shair [27] reported $\delta_H = 6.0\text{ (cal/cc)}^{1/2}$, that is, $12.37\text{ MPa}^{1/2}$, quoted as $12.3\text{ MPa}^{1/2}$ by LaPack et al. [28], at an unspecified temperature, a value comparable to some other reports. Span and Wagner [48] reported data over a wide temperature range for both the molar enthalpy and the density of the condensed and gaseous phases, from which the expression shown in Table 3 is derived for temperatures between the triple point $T_t = 216.59\text{ K}$ and $T = 298.15\text{ K}$, from which $\delta_H(T_t)/\text{MPa}^{1/2} = 19.10$ and $\delta_H(298.15\text{ K})/\text{MPa}^{1/2} = 6.78$ result, a wide span of values. Politzer et al. [49] predicted from ab initio computations for CO_2 the heats of formation at 298.15 K as $\Delta_f H/\text{kcal mol}^{-1} = -92.3$ for the gas and -96.6 for the liquid, yielding $\Delta_v H/\text{J mol}^{-1} = 17991$ for the difference, that is, for vaporization of the liquid. With the density at $T_t = 1.17846\text{ g cm}^{-3}$ this yields $\delta_H(T_t)/\text{MPa}^{1/2} = 20.82$. Prausnitz and Shair [27] quote Hansen [2] and report $\delta_d = 15.7\text{ MPa}^{1/2}$ at 298 K and 1 atm for the dispersion partial solubility parameter, but the total, Hildebrand solubility parameter included a contribution from the polar interactions and hydrogen bonding of this gas molecules, adding up to $\delta_H(298\text{ K})\text{MPa}^{1/2} = 17.85$. This value is incompatible with that resulting from the Span and Wagner data. It appears that the compilation of Span and Wagner [48] results in the most reliable values of $\delta_H(T)$ and that $\delta_H(T_t)/\text{MPa}^{1/2} = 19.10$ may be selected here.

2.1.14. Phosgene. The normal boiling point of COCl_2 was established as 280.66 K by Giauque and Jones [50] and was listed in the Handbook [7] as 8°C , that is, 281.2 K , and the most recently reported vapor pressure data of Huang et al. [51] lead to $T_b/\text{K} = 282.95$ at which the pressure equals 0.101325 MPa (i.e., 1 atm). The molar enthalpy of vaporization at the boiling point was reported as $\Delta_v H(T_b)/\text{cal mol}^{-1} = 5832 \pm 6$, that is, 24401 J mol^{-1} [50]. The more recent value [51] is larger, 25565 J mol^{-1} , derived from the vapor pressure curve. The density of liquid phosgene was reported by Davies [52] as $\rho/\text{g cm}^3 = 1.42014 - 0.0023120(t/^\circ\text{C}) - 0.000002872(t/^\circ\text{C})^2$, that is, $\rho(T_b)/\text{g cm}^3 = 1.40146$ and $V(T_b)/\text{cm}^3\text{ mol}^{-1} = 70.59$. A slightly smaller value, $70.13\text{ cm}^3\text{ mol}^{-1}$ results from the interpolated liquid density data in [51]. The solubility parameter resulting from the more recent $\Delta_v H$ is $\delta_H(T_b)\text{MPa}^{1/2} = 18.13$ and the temperature dependence is shown in Table 3.

2.1.15. Nitrogen Trifluoride. There are conflicting reports regarding the boiling point of liquid NF_3 : the older value is -119°C by Ruff et al. [53] and a more recent one is 144.2 K by Sladkov and Novikova [54], confirmed as -128.75°C [7], that is, $T_b = 144.40\text{ K}$, that is taken to be the valid one. Also, the reported $\Delta_v H$ values differ: 2400 cal mol^{-1} , that is, 10042 J mol^{-1} [53] and 11600 J mol^{-1} [54] or 11560 J mol^{-1} [7], and again the latter value is used. The molar volume at the boiling point is listed as $V(T_b) = 46.1\text{ cm}^3\text{ mol}^{-1}$ [54], so that $\delta_H(T_b)/\text{MPa}^{1/2} = 15.0$.

2.1.16. Nitrous Oxide. Yosim and Owens [21] used the $\Delta_v H$ data of Kelley and King [40] for N_2O , from which the value $\delta_H(T_b)\text{MPa}^{1/2} = 20.41$ is derived. Atake and Chihara [55] reported $\Delta_v H/\text{J mol}^{-1} = 16544$ and with the density data of Leadbetter et al. [56] yielding $V(T_b) = 35.64\text{ cm}^3\text{ mol}^{-1}$ this produced $\delta_H(T_b)/\text{MPa}^{1/2} = 20.52$. Sistla et al. [36] quote Hansen [2] and report $\delta_d = 11.5\text{ MPa}^{1/2}$ at 298 K and 1 atm for the dispersion partial solubility parameter, but the total, Hildebrand solubility parameter included a contribution from the polar interactions of these gas molecules, adding up to $\delta_H(298\text{ K})\text{MPa}^{1/2} = 20.81$. The average of these agreeing values, 20.58 ± 0.20 , is selected here.

2.1.17. Nitrogen Monoxide. Monomeric nitrogen oxide, NO , has received very little attention in the literature regarding its molar enthalpy of vaporization. A very early "calculated" value of 3412 cal mol^{-1} due to Bingham [57], that is, 14276 J mol^{-1} , differs from the value 3293 cal mol^{-1} , that is, 13778 J mol^{-1} of Kelley and King [40] quoted by Yosim and Owens [21]. From the latter, with the supplied density of 1.269 g cm^{-3} at the boiling point of 121.4 K , the solubility parameter $\delta_H(T_b)/\text{MPa}^{1/2} = 23.24$ is derived. There seems to be no more modern value for this quantity in the literature.

2.1.18. Silicon Tetrafluoride. The liquid range of SiF_4 (also called tetrafluorosilane) is quite narrow and its normal boiling point has been reported differently by various authors: $177.5 \leq T_b/\text{K} \leq 187.2$ [58], and its triple point, $T_t/\text{K} = 186.35$

[59]; hence, the lower values appear not to be valid. The higher values, 187 [60] and 187.2 [7], appear to be more nearly correct. The molar enthalpy of vaporization was reported by Lyman and Noda [61] as $15.802 \text{ kJ mol}^{-1}$ (but they report $T_b = 177.83 \text{ K}$, below T_t of 186.35 K , but discuss properties of the liquid!). The density of liquid SiF_4 was reported by Pace and Mosser [59] as $\rho/\text{g cm}^{-3} = 2.479 - 0.004566T$ at $186 \leq T/\text{K} \leq 195$, extrapolating to 1.624 g cm^{-3} at $T_b = 187.2 \text{ K}$ and a molar volume $V(T_b) = 64.08 \text{ cm}^3 \text{ mol}^{-1}$. The solubility parameter of SiF_4 is therefore $\delta_H(T_b)/\text{MPa}^{1/2} = 14.91$.

2.1.19. Sulfur Tetrafluoride. The data needed for obtaining the solubility parameter of SF_4 at its boiling point are all available from Brown and Robinson [68]. The boiling point is -40.4°C , that is, $T_b = 232.75 \text{ K}$, the molar enthalpy of vaporization is $6320 \text{ cal mol}^{-1}$, that is, 26443 J mol^{-1} , and the density of the liquid follows $\rho/\text{g cm}^{-3} = 2.5471 - 0.00314T$ (at $170 \leq T/\text{K} \leq 200$), assumed to be valid up to T_b , yielding $\rho(T_b)/\text{g cm}^{-3} = 1.8164$. Hence, $\delta_H(T_b)/\text{MPa}^{1/2} = 20.31$. A somewhat larger value of $T_b = 236 \text{ K}$ was reported later by Streng [69] with $\rho(T_b)/\text{g cm}^{-3} = 1.8061$, but with no other latent heat of vaporization. The resulting $\delta_H(T_b)/\text{MPa}^{1/2} = 20.22$ does not differ much from the value selected here.

2.1.20. Sulfur Hexafluoride. Since SF_6 sublimates and does not form a liquid on heating the solid; it is difficult to specify a temperature at which the solubility parameter should be obtained. The triple point has been reported as $T_t = 223.56 \text{ K}$ by Funke et al. [70], but the molar enthalpy of vaporization and the density have been reported at other temperatures. Linford and Thornhill [24] reported the molar energy of vaporization as $4.08 \text{ kcal mol}^{-1}$, that is, 17071 J mol^{-1} , at an unspecified temperature. A so-called “boiling temperature” of 204 K was reported by Gorbachev [71] at which the molar volume of SF_6 was $75.3 \text{ cm}^3 \text{ mol}^{-1}$. The value $\delta_H(204 \text{ K})/\text{MPa}^{1/2} = 14.29$ results from this pair of data. Funke et al. [70] reported vapor pressures and liquid densities over the temperature range 224 to 314 K . From these data the molar enthalpy of vaporization is $\Delta_v H = 17375 \text{ J mol}^{-1}$ and the molar volume is $V = 79.16 \text{ cm}^3 \text{ mol}^{-1}$ at 224 K , yielding $\delta_H(224 \text{ K})/\text{MPa}^{1/2} = 14.82$. However, a considerably larger $\Delta_v H = 5.6 \text{ kcal mol}^{-1}$ was quoted from Lange’s Handbook of Chemistry for SF_6 by Anderson et al. [72], that is, 23430 J mol^{-1} . This value is near the molar enthalpy of sublimation $\Delta_{\text{subl}} H = 23218 \text{ J mol}^{-1}$ at 186 K reported by Ohta et al. [73]. However, no density data at this temperature, lower than the triple point, are available. A tentative value, based on the data in [70], is suggested here $\delta_H(224 \text{ K})/\text{MPa}^{1/2} = 14.82$ as representative.

2.1.21. Diborane. The molar enthalpy of vaporization of B_2H_6 at the boiling point $T_b = 180.32 \text{ K}$ was reported by Clarke et al. [74] as $\Delta_v H/\text{cal mol}^{-1} = 3412$ in the text and as 3422 as the average of four runs in a table, that is, $14297 \pm 21 \text{ J mol}^{-1}$. The density was reported by Laubengayer et al. [75] as $\rho/\text{g cm}^{-3} = 0.3140 - 0.001296(t/^\circ\text{C})$, being accordingly 0.4343 at T_b , yielding a molar volume of $63.71 \text{ cm}^3 \text{ mol}^{-1}$ and a solubility parameter of $\delta_H(T_b)/\text{MPa}^{1/2} = 14.17$. A subsequent

study by Wirth and Palmer [76] reported $T_b = 180.63 \text{ K}$ and $\Delta_v H/\text{cal mol}^{-1} = 3413$, that is, 14280 J mol^{-1} . The molar volume at the boiling point $T_b = 180.66 \text{ K}$ was quoted by Jhon et al. [77] from the Landolt-Börnstein compilation as $63.36 \text{ cm}^3 \text{ mol}^{-1}$. This pair of values yields $\delta_H(T_b)/\text{MPa}^{1/2} = 14.20$. The average between the two values, 14.185 , is selected here.

2.1.22. Silane. The boiling point and molar heat of vaporization of liquid SiH_4 were quoted by Taft and Sisler [78] from secondary sources as 161 K and $2.98 \text{ kcal mol}^{-1}$, that is, 12470 J mol^{-1} , and listed in [7] as -111.9°C , that is, 161.3 K and 12.1 kJ mol^{-1} . The molar volume at the boiling point was reported by Zorin et al. [79] from experimental density measurements as $V(T_b) = 55.04 \text{ cm}^3 \text{ mol}^{-1}$ and from molecular dynamics simulations of the density reported by Sakiyama et al. [80] interpolated to the boiling point as $V(T_b) = 57.27 \text{ cm}^3 \text{ mol}^{-1}$, but the experimental value is preferred. The resulting solubility parameter is $\delta_H(T_b)/\text{MPa}^{1/2} = 14.22$.

2.1.23. Germane. The boiling point and molar heat of vaporization of liquid GeH_4 were quoted in [78] from secondary sources as 184 K and $3.65 \text{ kcal mol}^{-1}$, that is, 15270 J mol^{-1} , reported by Devyatikh et al. [81] as -88.51°C and $3608 \text{ cal mol}^{-1}$, that is, 15096 J mol^{-1} , and listed in [7] as -88.1°C , that is, 185.05 K and $14.06 \text{ kJ mol}^{-1}$. The molar volume at the boiling point was reported in [79] from experimental density measurements as $V(T_b) = 55.91 \text{ cm}^3 \text{ mol}^{-1}$. Hence $\delta_H(T_b)/\text{MPa}^{1/2} = 14.97$ results from the more recent data.

2.1.24. Stannane. There are only the older data for liquid SnH_4 ; the boiling point and molar heat of vaporization were reported by Paneth et al. [82] as -52°C and $4.55 \text{ kcal mol}^{-1}$ and were quoted in [78] from secondary sources as 221 K and $4.5 \text{ kcal mol}^{-1}$, that is, 18800 J mol^{-1} . The molar volume at the boiling point was reported in [79] from experimental density measurements as $V(T_b) = 63.18 \text{ cm}^3 \text{ mol}^{-1}$. Hence $\delta_H(T_b)/\text{MPa}^{1/2} = 16.40$ results.

2.1.25. Phosphine. The paper by Durrant et al. [83] reports all the required data for the group V hydrides. For PH_3 the boiling points -87.4 , -85 , and -86.2°C were quoted in [83] from previous publications, 187 K is listed in [78], -87.9°C is reported by Devyatikh et al. [81], and -87.75°C is listed in [7], that is, $T_b = 185.40 \text{ K}$, which is taken as the valid value. The molar enthalpy of vaporization at the boiling point is reported as $\Delta_v H(T_b) = 3.85 \text{ kcal mol}^{-1}$ in [83], that is, 16110 J mol^{-1} , as $3.79 \text{ kcal mol}^{-1}$ in [55], that is, 15860 J mol^{-1} , as $3.949 \text{ kcal mol}^{-1}$ in [81], that is, 16520 J mol^{-1} . However, considerably lower values were reported more recently: 14600 J mol^{-1} in [7] and 13440 J mol^{-1} in [84] as the measured value. (Note that Ludwig [84] reports for H_2S an experimental $\Delta_v H$ value in accord with other reports, so that it is unclear why for PH_3 such a low value is reported.) The mean of the earlier reported values, namely, $\Delta_v H(T_b)/\text{J mol}^{-1} = 16160$, is taken as valid. The density of PH_3 at the boiling point

is interpolated in the data of [83] as $\rho(T_b) = 0.7653 \text{ g cm}^{-3}$ yielding $V(T_b) = 44.43 \text{ cm}^3 \text{ mol}^{-1}$. A somewhat larger value, $V(T_b) = 45.72 \text{ cm}^3 \text{ mol}^{-1}$ was reported in [79]. The solubility parameters $\delta_H(T_b)/\text{MPa}^{1/2} = 18.13$ and 17.88 result from these two molar volume values, and the mean, 18.00 , is selected here.

2.1.26. Arsine. Durrant et al. [83] report the boiling point of liquid AsH_3 as 214.5 K in agreement with some earlier data but somewhat lower than a much older value, 218.2 , quoted also in [78] and larger than the value 211.1 K (from -62.1°C) reported in [81]. Sherman and Giauque [85] report $T_b = 210.68 \text{ K}$, listed as -62.5°C in [7], that is, 210.65 K , and a mean $\Delta_v H(T_b) = 3988 \text{ cal mol}^{-1}$, that is, 16686 J mol^{-1} . The molar enthalpy of vaporization at the boiling point is reported as $\Delta_v H(T_b) = 4.34 \text{ kcal mol}^{-1}$ in [83], that is, 18160 J mol^{-1} , as $4.27 \text{ kcal mol}^{-1}$ in [78], that is, 17870 J mol^{-1} , as $4.100 \text{ kcal mol}^{-1}$ in [81], that is, 17150 J mol^{-1} . Again, a lower value, 16690 J mol^{-1} , is listed in [7], but the average of the former three values, 17730 J mol^{-1} , is taken here as valid. The density of AsH_3 at the boiling point is interpolated in the data of [83] as $\rho(T_b) = 1.6320 \text{ g cm}^{-3}$ yielding $V(T_b) = 47.76 \text{ cm}^3 \text{ mol}^{-1}$. A very similar value, $47.82 \text{ cm}^3 \text{ mol}^{-1}$, was reported in [79]. The resulting solubility parameter is $\delta_H(T_b)/\text{MPa}^{1/2} = 18.27$.

2.1.27. Stibine. Durrant et al. [83] report the boiling point of liquid SbH_3 as -17.0°C , that is, 256.2 K , in agreement with 256 K in [78]. The molar enthalpy of vaporization at the boiling point is reported as $\Delta_v H(T_b) = 5.067 \text{ kcal mol}^{-1}$ in [83], that is, 21200 J mol^{-1} , and as 4.9 to $5.0 \text{ kcal mol}^{-1}$ in [78], that is, 20700 J mol^{-1} , and is listed as 21300 J mol^{-1} in [7]; the latter is taken as valid. The density of AsH_3 at the boiling point is interpolated in the data of [83] as $\rho(T_b) = 2.2039 \text{ g cm}^{-3}$ yielding $V(T_b) = 56.62 \text{ cm}^3 \text{ mol}^{-1}$. A larger value, $57.83 \text{ cm}^3 \text{ mol}^{-1}$, was reported in [79]. The resulting solubility parameters are $\delta_H(T_b)/\text{MPa}^{1/2} = 18.40$ and 18.20 , their mean, 18.30 , being selected here.

2.1.28. Hydrogen Sulfide. The molar enthalpy of vaporization of H_2S was reported by Cubitt et al. [86] from experimental data as $\Delta_v H = 18701 \text{ J mol}^{-1}$ and the molar volume as $V = 35.83 \text{ cm}^3 \text{ mol}^{-1}$ (interpolated) at the boiling point $T_b = 212.85 \text{ K}$. The value $\delta_H(T_b)/\text{MPa}^{1/2} = 21.74$ results from these values. The temperature dependence of δ_H is shown in Table 3. A less precise value of $\Delta_v H = 18.36 \text{ kJ mol}^{-1}$ and a density of $\rho = 934 \text{ kg m}^{-3}$ were reported as experimental values at 220.2 K from an undisclosed source by Kristóf and Liszi [87]. The value $\delta_H(220.2 \text{ K})/\text{MPa}^{1/2} = 21.28$ is derived from these data. $\Delta_v H = 18.67 \text{ kJ mol}^{-1}$ at the boiling point was reported by Ludwig [84] as the experimental value. A value $\Delta_v H = 4.46 \text{ kcal mol}^{-1}$, that is, 18661 J mol^{-1} at the boiling point, was reported by Riahi and Rowley [88] as well as by Orabi and Lamoureux [89], attributed to Clarke and Glew [90], and the density 949 kg m^{-3} and a density of 940 kg m^{-3} result from the data of [79]. These values yield $\delta_H(T_b)/\text{MPa}^{1/2} = 21.69$. Sistla et al. [36] quote Hansen

[2] and report $\delta_d = 17.0 \text{ MPa}^{1/2}$ at 298 K and 1 atm for the dispersion partial solubility parameter, but the total, Hildebrand solubility parameter included a contribution from the polar interactions of these gas molecules, adding up to $\delta_H(298 \text{ K})/\text{MPa}^{1/2} = 20.71$. The average of the values resulting from [86, 89], $\delta_H(T_b)/\text{MPa}^{1/2} = 20.72$, nearly coincides with the latter value (for 298 K).

2.1.29. Hydrogen Selenide. The boiling point of H_2Se was reported as -41.5°C by Robinson and Scott [91], 231 K in [78], taken from secondary sources, and as -41.25°C in [7], that is, 231.90 K . The very early $\Delta_v H(T_b) = 4740 \text{ cal mol}^{-1}$ by Forcrand and Fonze-Diacon [92] at the boiling point -42°C , that is, 19830 J mol^{-1} , is confirmed by the value 19790 J mol^{-1} , derived from the Trouton constant of $20.4 \text{ cal K}^{-1} \text{ mol}^{-1}$ reported in [91], leading to $4.78 \text{ kcal mol}^{-1}$ in [78], that is, 20000 J mol^{-1} . The $\rho(T_b) = 2.004 \text{ g cm}^{-3}$ [91] yields $V(T_b) = 40.42 \text{ cm}^3 \text{ mol}^{-1}$. The density data of [79] yield the reported $V(T_b) = 41.21 \text{ cm}^3 \text{ mol}^{-1}$; hence, the solubility parameter $\delta_H(T_b)/\text{MPa}^{1/2} = 20.97$ results from the means of the $\Delta_v H(T_b)$ and $V(T_b)$ values.

2.1.30. Hydrogen Telluride. Robinson and Scott [91] reported boiling points of -4 and -5°C , definitely lower than previous reports leading to 272 K in [78] and -2°C in [7]. For the present purpose $T_b = 270 \text{ K}$ is used. Trouton's constant $16.7 \text{ cal K}^{-1} \text{ mol}^{-1}$ reported in [91] yields $\Delta_v H(T_b) = 18870 \text{ J mol}^{-1}$, much lower than 23430 J mol^{-1} (from $5.6 \text{ kcal mol}^{-1}$) from [78], but confirmed by 19.2 kJ mol^{-1} listed in [7]. The mean, 19040 J mol^{-1} , of the better agreeing values is used here. The density at the boiling point is 2.650 g cm^{-3} according to [91], yielding $V(T_b) = 48.9 \text{ cm}^3 \text{ mol}^{-1}$, much lower than $55.14 \text{ cm}^3 \text{ mol}^{-1}$ resulting from the density data in [79]. The minimal value of $\delta_H(T_b)/\text{MPa}^{1/2}$ from these data is 17.5 and the maximal value is 20.8 . The value $18.4 \text{ MPa}^{1/2}$ from the old data of [91] may represent the true value, but the trend with the molar mass of the gaseous substances points to the maximal value $20.8 \text{ MPa}^{1/2}$ as possibly better.

2.1.31. Methane. Yosim and Owens [21] used the $\Delta_v H$ data of Kelley and King [40], from which the value $\delta_H(T_b)/\text{MPa}^{1/2} = 13.83$ is derived. Prausnitz and Shair [27] reported $\delta_H = 5.68 (\text{cal/cc})^{1/2}$, that is, $11.62 \text{ MPa}^{1/2}$ (reported as 11.6 in [28]), a low value compared to other reports. Linford and Thornhill [24] reported the energy of vaporization as $\Delta_v E(T_b) = 1.73 \text{ kcal mol}^{-1}$ and with the molar volume from Terry et al. [30], $V(T_b) = 38.1 \text{ cm}^3 \text{ mol}^{-1}$, the value $\delta_H(T_b) = 12.87 \text{ MPa}^{1/2}$ is derived. Jorgensen et al. [93] quoted experimental data at the boiling point from compilations: $\Delta_v H/\text{kcal mol}^{-1} = 1.96$ and $V/\text{\AA}^3 \text{ molecule}^{-1} = 62.8$, from which $\delta_H(T_b)/\text{MPa}^{1/2} = 13.86$ is calculated. Daura et al. [94] quoted experimental data at the boiling point from compilations: $\Delta_v H/\text{kJ mol}^{-1} = 8.19$ and density $\rho/\text{kg m}^{-3} = 424$, from which $\delta_H(T_b)/\text{MPa}^{1/2} = 13.87$ is calculated. Prausnitz and Shair [27] quote Hansen [2] and report $\delta_d = 14.0 \text{ MPa}^{1/2}$ at 298 K and 1 atm for the

dispersion partial solubility parameter, which for methane is the total solubility parameter. The mean of the agreeing values, $\delta_H(T_b)/\text{MPa}^{1/2} = 13.87$ is selected here.

2.1.32. Fluoromethane. Oi et al. [95] provided the coefficients of the vapor pressure expression $\log(p/\text{torr}) = A - B/(C + t/^\circ\text{C})$ for CH_3F , from which $\Delta_v H(T_b) = 15764 \text{ J mol}^{-1}$ is derived. Fonseca and Lobo [96] provided the molar volume of CH_3F at 161.39 K and at 195.48 K, from which $V(T_b = 194.8 \text{ K}) = 38.61 \text{ cm}^3 \text{ mol}^{-1}$ is interpolated. The resulting solubility parameter is $\delta_H(T_b)/\text{MPa}^{1/2} = 19.14$.

2.1.33. Difluoromethane. Potter et al. [97] provided the needed data for the calculation of the solubility parameter: $p(T)/\text{bar}$, $\rho(T)/\text{g cm}^{-3}$, and $\Delta_v H(T)/\text{kJ mol}^{-1}$, from the former of which $T_b = 221.6 \text{ K}$ is interpolated for $p/\text{bar} = 1.01325$ ($= 1 \text{ atm}$ for the normal boiling point). The resulting values $\rho(T_b)/\text{g cm}^{-3} = 1.268$ and $\Delta_v H(T_b)/\text{kJ mol}^{-1} = 19.97$ yield $\delta_H(T_b)/\text{MPa}^{1/2} = 21.02$ for CH_2F_2 . The temperature dependence of δ_H is shown in Table 3.

2.1.34. Trifluoromethane. Potter et al. [97] provided the needed data for the calculation of the solubility parameter: $p(T)/\text{bar}$, $\rho(T)/\text{g cm}^{-3}$, and $\Delta_v H(T)/\text{kJ mol}^{-1}$, from the former of which $T_b = 191.1 \text{ K}$ is interpolated. The resulting values $\rho(T_b)/\text{g cm}^{-3} = 1.467$, and $\Delta_v H(T_b)/\text{kJ mol}^{-1} = 16.14$ yield $\delta_H(T_b)/\text{MPa}^{1/2} = 17.46$ for CHF_3 . The temperature dependence of δ_H is shown in Table 3.

2.1.35. Tetrafluoromethane. Gilmour et al. [98] reported the values of $T_b = 145.1 \text{ K}$, $\Delta_v H(T_b)/\text{kcal mol}^{-1} = 3.01$ ($= 12.59 \text{ kJ mol}^{-1}$), and $V(T_b)/\text{cm}^3 \text{ mol}^{-1} = 54.9$, from which $\delta_H(T_b) = 14.40 \text{ MPa}^{1/2}$ results. Linford and Thornhill [24] reported the energy of vaporization as $\Delta_v E(T_b) = 2.72 \text{ kcal mol}^{-1}$ at $T_b = 145.2 \text{ K}$ and with the molar volume from Terry et al. [30], $V(T_b) = 54.4 \text{ cm}^3 \text{ mol}^{-1}$, the value $\delta_H(T_b) = 14.46 \text{ MPa}^{1/2}$ is derived. The values resulting from the Potter et al. [97] data are $\rho(T_b)/\text{g cm}^{-3} = 1.563$ and $\Delta_v H(T_b)/\text{kJ mol}^{-1} = 11.72$, yielding $\delta_H(T_b)/\text{MPa}^{1/2} = 14.66$. The most recent report is of Monte Carlo computer simulation results by Watkins and Jorgensen [99] that compare well with the experimental values for the enthalpy of vaporization and the density, yielding $\delta_H(T_b)/\text{MPa}^{1/2} = 14.48$. The mean of the three closely agreeing reported values, $14.43 \text{ MPa}^{1/2}$, is taken to represent the solubility parameter of CF_4 . The temperature dependence of δ_H is shown in Table 3.

2.1.36. Chloromethane. Meyer et al. [100] reported the coefficients of the Antoine vapor pressure expression [missing the minus sign between A and $B/(C + t)$ for $\log p$], from which was obtained $\Delta_v H/\text{kJ mol}^{-1} = 22803$ over the range $-75 \leq t/^\circ\text{C} \leq -25$, that is, up to the boiling point of -24.14°C , that is, 249.0 K . Kumagai and Iwasaki [101] reported the specific volumes of CH_3Cl at the saturated vapor pressures at four temperatures above -20°C , extrapolating to $0.988 \text{ cm}^3 \text{ g}^{-1}$ at T_b and a molar volume of $49.40 \text{ cm}^3 \text{ mol}^{-1}$. The value $\delta_H(T_b)/\text{MPa}^{1/2} = 20.38$ results from these data. Freitas et

al. [102] quoted $\Delta_v H(T_b)/\text{kJ mol}^{-1} = 21.5$ and the density $\rho/\text{g cm}^{-3} = 0.985$ from a secondary source, taking $T_b = 239.39 \text{ K}$. The resulting solubility parameter is $\delta_H(T_b)/\text{MPa}^{1/2} = 19.47$. The mean of the two values, $19.9 \text{ MPa}^{1/2}$, is taken for the solubility parameter for CH_3Cl .

2.1.37. Bromomethane. The boiling point $T_b = 276.70 \text{ K}$ of CH_3Br and its molar enthalpy of vaporization at this temperature $\Delta_v H(T_b) = 5.76 \text{ kcal mol}^{-1}$ ($= 24.10 \text{ kJ mol}^{-1}$) were reported by Kudchadker et al. [103]. The specific volumes at $-20, 0, 20$, and 40°C and saturation pressures were reported by Kumagai and Iwasaki [101], yielding a linear relationship. From which the density $\rho(T_b)/\text{g cm}^{-3} = 1.7196$ and the molar volume $V(T_b)/\text{cm}^3 \text{ mol}^{-1} = 55.21$ could be derived. The resulting solubility parameter is $\delta_H(T_b)/\text{MPa}^{1/2} = 19.87$.

2.1.38. Formaldehyde. The boiling point of liquid HCHO was reported as -21.5°C by Mali and Ghosh [104], that is, 252 K . The density at -20°C of 0.815 g cm^{-3} is available in [7]. The latent heat of evaporation was reported as $5600 \text{ cal mol}^{-1}$ in [104]. The resulting solubility parameter is $\delta_H(T_b)/\text{MPa}^{1/2} = 24.06$. These are the only data found for this gaseous substance in the neat liquid form; hence the value of δ_H must be considered as tentative.

2.1.39. Methylthiol. The molar enthalpy of vaporization of CH_3SH was reported by Russell et al. [105] as $5872 \text{ cal mol}^{-1}$, that is, 24568 J mol^{-1} , at the normal boiling point $T_b = 279.12 \text{ K}$. The density was reported by Kaminski et al. [106] presumably at T_b (for which the above-noted reference is appropriate) as 0.888 g cm^{-3} . Hence, the solubility parameter is $\delta_H(T_b)/\text{MPa}^{1/2} = 20.26$.

2.1.40. Acetylene. This substance sublimates and has no definite liquid phase at ambient pressures, hence no boiling point. The triple point T_t was reported as 192.4 K by Tan et al. [107] and the molar volume at 191.9 K was reported as $42.06 \text{ cm}^3 \text{ mol}^{-1}$ from molecular dynamics computation by Klein and McDonald [108]. These authors also deduced the molar enthalpy of vaporization over the temperature range of 191 to 223 K from vapor pressure data of Kordes [109] as 16.6 kJ mol^{-1} , who also reported the density at 191.5 K as 0.613 g cm^{-3} , that is, $V(T_b) = 42.48 \text{ cm}^3 \text{ mol}^{-1}$. The resulting solubility parameter of $\text{HC}\equiv\text{CH}$ is thus $\delta_H(T_t) = 18.89 \text{ MPa}^{1/2}$. According to Vitovec and Fried [65], quoting from a secondary source, under pressure (48 atm) at 25°C the enthalpy of vaporization of the saturated acetylene is $3.737 \text{ kcal mol}^{-1}$ and the molar volume is $69.14 \text{ cm}^3 \text{ mol}^{-1}$, yielding $\delta_H(298 \text{ K}) = 6.75 \text{ cal}^{1/2} \text{ cm}^{-3/2}$, that is, $13.81 \text{ MPa}^{1/2}$. The solubility of acetylene in benzene, toluene, and *p*-xylene at 25°C [65] and application of the regular solution expression $\ln x_{\text{HCCH}} = -(V_{\text{HCCH}}/RT)[\delta_H(\text{HCCH}) - \delta_H(\text{solvent})]^2$ yielded the mean value $6.86 \text{ cal}^{1/2} \text{ cm}^{-3/2}$, that is, $14.03 \text{ MPa}^{1/2}$, for $\delta_H(\text{HCCH})$, in fair agreement with their value from the enthalpy of vaporization. Sistla et al. [36] quote from Hansen [2] values for the dispersion, polar, and hydrogen bonding partial solubility parameters of $14.4, 4.2$, and $11.9 \text{ MPa}^{1/2}$, respectively, adding

up to the total $\delta_H(298\text{ K}, 1\text{ atm}) = 19.15\text{ MPa}^{1/2}$, an unlikely value in view of the nonexistence of liquid acetylene at 298 K and 1 atm.

2.1.41. Ethylene. Prausnitz and Shair [27] reported $\delta_H = 6.6\text{ (cal/cc)}^{1/2}$, that is, $13.5\text{ MPa}^{1/2}$, a low value compared to other reports. Michels and Wassenaar [110] reported an expression for the temperature dependence of the vapor pressure, leading to $\Delta_v H(T) = 14.641\text{ kJ mol}^{-1}$ ($148 \leq T/\text{K} \leq 281$). Yosim and Owens [21] used the density and $\Delta_v H$ data from a secondary source, from which the value $\delta_H(T_b)\text{ MPa}^{1/2} = 15.64$ is derived. Calado et al. [111] reported liquid molar volumes and enthalpies of vaporization over the temperature range $110 \leq T \leq 250$, from which the values at the boiling point of C_2H_4 $T_b = 169.5\text{ K}$ of $V(T_b)/\text{cm}^3\text{ mol}^{-1} = 49.48$ and $\Delta_v H(T_b)/\text{J mol}^{-1} = 13447$ are deduced, yielding $\delta_H(T_b)/\text{MPa}^{1/2} = 15.60$. The temperature dependence of δ_H is shown in Table 3. Sistla et al. [36] quote from Hansen [2] values for the dispersion, polar, and hydrogen bonding partial solubility parameters of 15.0, 2.7, and 2.7 $\text{MPa}^{1/2}$, respectively, adding up to the total $\delta_H(298\text{ K}, 1\text{ atm}) = 15.48\text{ MPa}^{1/2}$. The value from Calado et al. [111] is selected here as valid.

2.1.42. Ethane. Prausnitz and Shair [27] reported $\delta_H = 6.6\text{ (cal/cc)}^{1/2}$, that is, $13.5\text{ MPa}^{1/2}$, repeated in [28], a low value compared to other reports. Yosim and Owens [21] used the density and $\Delta_v H$ data from a secondary source, from which the value $\delta_H(T_b)\text{ MPa}^{1/2} = 14.56$ is derived. Bradford and Thodos [66] reported expressions and parameters from which the solubility parameter was supposed to be calculated, but the resulting value ($7.9\text{ MPa}^{1/2}$) is too small. Gilmour et al. [98] reported density and $\Delta_v H$ data from an undisclosed source, from which the value $\delta_H(T_b)\text{ MPa}^{1/2} = 15.5$ is deduced. Linford and Thornhill [24] reported the energy of vaporization as $\Delta_v E(T_b) = 3.15\text{ kcal mol}^{-1}$ and with the density of $\rho(T_b) = 0.5481\text{ g cm}^{-3}$ extrapolated from the data of Chui and Canfield [112], the value $\delta_H(T_b) = 15.50\text{ MPa}^{1/2}$ is derived. Jorgensen et al. [93] reported the molecular volume in $\text{\AA}^3\text{ molecule}^{-1}$ of ethane at its boiling point, from which the molar volume $55.1\text{ cm}^3\text{ mol}^{-1}$ is obtained, that with the $\Delta_v H(T_b) = 3.52\text{ kcal mol}^{-1}$ that they report yields $\delta_H(T_b)\text{ MPa}^{1/2} = 15.48$. Daura et al. [94] report $\Delta_v H(T_b) = 14.70\text{ kJ mol}^{-1}$ and the density $\rho(T_b) = 0.546\text{ kg m}^{-3}$, from which $\delta_H(T_b)\text{ MPa}^{1/2} = 15.48$ results. Sistla et al. [36] quote Hansen [2] and report $\delta_d = 15.6\text{ MPa}^{1/2}$ at 298 K and 1 atm for the dispersion partial solubility parameter, which for ethane is the total solubility parameter. The value $\delta_H(T_b) = 15.50\text{ MPa}^{1/2}$ is selected here.

2.1.43. Chloroethane. The boiling point of $\text{C}_2\text{H}_5\text{Cl}$ is somewhat below ambient, $12.26^\circ\text{C} = 285.4\text{ K}$, and the coefficients of the Antoine vapor pressure expression [missing the minus sign between A and $B/(C + t)$ for $\log p$] were reported by Meyer et al. [100], from which $\Delta_v H/\text{kJ mol}^{-1} = 26.615$ was obtained over the range $-56 \leq t/^\circ\text{C} \leq 13$. A somewhat smaller $\Delta_v H/\text{kJ mol}^{-1} = 24.73$ was quoted by Smith [113] from a secondary source. The molar volume was estimated by

Taft et al. [114] (for an unspecified temperature, presumably 25°C) as $V = 71.5\text{ cm}^3\text{ mol}^{-1}$, whereas the Handbook [7] specifies the density as $\rho(25^\circ\text{C}) = 0.8902\text{ g cm}^{-3}$, from which the molar volume is $V(25^\circ\text{C}) = 69.1\text{ cm}^3\text{ mol}^{-1}$. Averaging the $\Delta_v H$ and V values, the tentative solubility parameter is $18.2\text{ MPa}^{1/2}$ near the boiling point.

2.1.44. Hexafluoroethane. Gilmour et al. [98] provided the molar enthalpy of vaporization (from vapor pressure measurements) and the molar volume of C_2F_6 at the boiling point 194.9 K , yielding the value $\delta_H(T_b) = 13.00\text{ MPa}^{1/2}$ and reported $\delta_H/\text{cal}^{1/2}\text{ cm}^{-3/2} = 6.4$, that is, $13.1\text{ MPa}^{1/2}$ (with the error of inverting the signs on the units). Subsequently Watkins and Jorgensen [99] quoted literature values of the molar enthalpy of vaporization and the density of C_2F_6 at the boiling point 195.05 K , yielding the value $\delta_H(T_b) = 12.94\text{ MPa}^{1/2}$. Sharafi and Boushehri [115] reported the following values: $T_b = 194.95\text{ K}$, $\rho(T_b) 1605\text{ kg m}^{-3}$, and $\Delta_v H(T_b)/R = 1942.2\text{ K}$, from which $\delta_H(T_b) = 13.00\text{ MPa}^{1/2}$ is derived. The mean, $12.98\text{ MPa}^{1/2}$, is selected here.

2.1.45. Ethylene Oxide. Maass and Boomer [116] measured the vapor pressure and density of $c\text{-C}_2\text{H}_4\text{O}$ over a considerable temperature range and reported the molar enthalpy of vaporization at the boiling point, -10.73°C (283.88 K), as $\Delta_v H(T_b)/\text{kcal K}^{-1}\text{ mol}^{-1} = 6.00$, that is, 25104 J mol^{-1} . At this temperature (interpolated) the density is 0.8823 g cm^{-3} and the molar volume is $49.93\text{ cm}^3\text{ mol}^{-1}$. The resulting solubility parameter is $\delta_H(T_b) = 21.34\text{ MPa}^{1/2}$. Giauque and Gordon [117] obtained $\Delta_v H(T_b)/\text{kcal mol}^{-1} = 6.101$ calorimetrically (6.082 from the vapor pressures), that is, 25527 J mol^{-1} . Olson [118] reported the density at three temperatures: 0 , 25 , and 50°C , interpolated to $\rho(T_b) = 0.88266\text{ g cm}^{-3}$ and $V(T_b) = 49.91\text{ cm}^3\text{ mol}^{-1}$. These two data yield $\delta_H(T_b) = 21.55\text{ MPa}^{1/2}$. Eckl et al. [119] recently reported the density and molar enthalpy of vaporization at 235 , 270 , 305 , and 340 K , from which the interpolated values for $T_b = 283.5\text{ K}$ are $\Delta_v H(T_b)/\text{kJ mol}^{-1} = 25659$ and $\rho(T_b)/\text{mol L}^{-1} = 20.07$, that is, $V(T_b) = 49.83\text{ cm}^3\text{ mol}^{-1}$, resulting in $\delta_H(T_b) = 21.62\text{ MPa}^{1/2}$ and the temperature dependence is shown in Table 3. The mean of the latter two mutually agreeing estimates is selected here, $21.59\text{ MPa}^{1/2}$.

2.1.46. Dimethyl Ether. Maass and Boomer [116] measured the vapor pressure and density of $(\text{CH}_3)_2\text{O}$ over a considerable temperature range and reported the molar enthalpy of vaporization at the boiling point, -24.9°C (248.25 K), as $\Delta_v H(T_b)/\text{kcal K}^{-1}\text{ mol}^{-1} = 5.31$, that is, 22220 J mol^{-1} . At this temperature the (interpolated) density is 0.7345 g cm^{-3} and the molar volume is $62.72\text{ cm}^3\text{ mol}^{-1}$. The resulting solubility parameter is $\delta_H(T_b) = 17.93\text{ MPa}^{1/2}$. Kennedy et al. [120] measured the vapor pressure and reported the molar enthalpy of vaporization at the boiling point as $\Delta_v H(T_b)/\text{cal K}^{-1}\text{ mol}^{-1} = 5141.0$, that is, 21510 J mol^{-1} . Staveley and Tupman [121] reported the molar entropy of vaporization at the temperature at which the vapor pressure is 760 mmHg , that is, the boiling

point, $T_b = 248.4$ K. $\Delta_v S/\text{cal K}^{-1} \text{mol}^{-1} = 20.73$. Hence, the molar enthalpy of vaporization is $\Delta_v H/\text{kJ mol}^{-1} = T_b \Delta_v S = 21680$, near that reported in [120] and quoted by Briggs et al. [122], who reported the boiling point as -24.8°C . The mean of the latter two $\Delta_v H$ values and the Maass and Boomer [116] molar volume yield the solubility parameter $\delta_H(T_b) = 17.65 \text{ MPa}^{1/2}$, selected here instead of the slightly larger earlier value.

2.1.47. Propene. Powell and Giauque [123] reported vapor pressure data for C_3H_6 from which they derived the molar enthalpy of vaporization $4402 \text{ cal mol}^{-1}$, that is, 18418 J mol^{-1} , and reported the boiling point as 225.35 K. Jorgensen et al. [124] adopted this value for $\Delta_v H(T_b)/\text{cal K}^{-1} \text{mol}^{-1}$ at $T_b = 225.5$ K. The densities for propene under pressure were reported by Parrish [125] between 5 and 25°C that were extrapolated to 225.5 K as $\rho(T_b)/\text{g cm}^{-3} = 0.60049$ yielding $V(T_b) = 70.08 \text{ cm}^3 \text{mol}^{-1}$. The resulting solubility parameter is $\delta_H(T_b) = 15.36 \text{ MPa}^{1/2}$.

2.1.48. Cyclopropane. Ruehrwein and Powell [126] measured the vapor pressures of $c\text{-C}_3\text{H}_6$ and derived the molar enthalpy of vaporization $\Delta_v H(T_b)/\text{cal mol}^{-1} = 4793$, that is, 20054 J mol^{-1} , at the boiling point $T_b = 240.30$ K. Lin et al. [127] reported the molar enthalpy of vaporization at temperatures $\geq 20^\circ\text{C}$, obtained from the vapor pressures, extrapolating to $\Delta_v H(T_b)/\text{cal g}^{-1} = 119.03$, that is, 20956 J mol^{-1} . Calado et al. [111] reported a vapor pressure expression from which $\Delta_v H(T)/\text{kcal mol}^{-1} = 22200 \text{ J mol}^{-1}$ is calculated for $170 \leq T/\text{K} \leq 225$. Helgeson et al. [128] reported $\Delta_v H(T_b)/\text{kcal mol}^{-1} = 4.79$, that is, 20041 J mol^{-1} . The agreement between these values is only fair, and their mean, 20810 J mol^{-1} , is adopted here. The densities reported by Lin et al. [127] at temperatures $\geq 20^\circ$ extrapolate to 0.7119 g cm^{-3} at T_b , Helgeson et al. [128] reported 0.705 g cm^{-3} at T_b , and Costa Gomes et al. [129] report data up to 175 K that extrapolate to 689.4 kg m^{-3} at T_b . Again, the mean of these three values is adopted here, 0.7021 g cm^{-3} . The resulting solubility parameter is $\delta_H(T_b) = 17.7 \text{ MPa}^{1/2}$.

2.1.49. Propane. Linford and Thornhill [24] reported the energy of vaporization as $\Delta_v E(T_b) = 4.03 \text{ kcal mol}^{-1}$, that is, 16845 J mol^{-1} , and with the molar volume $V(T_b)/\text{\AA}^3 \text{molecule}^{-1} = 126.0$, that is, $75.88 \text{ cm}^3 \text{mol}^{-1}$, from Jorgensen et al. [93], the value $\delta_H(T_b) = 14.90 \text{ MPa}^{1/2}$ is derived. The latter authors provided $\Delta_v H(T_b)/\text{kcal mol}^{-1} = 4.49$, that is, 18686 J mol^{-1} at the boiling point $T_b = 231.88$ K, so that the same value $\delta_H(T_b) = 14.90 \text{ MPa}^{1/2}$ is derived. Bradford and Thodos [66] reported the parameters of the following expression:

$$\delta_H = \delta_c + k(1 - T_R)^m, \quad (5)$$

where $\delta_c = 2.362 (\text{cal/cm}^3)^{1/2}$ is the solubility parameter at the critical point, $k = 7.45$, $m = 0.446$, and $T_R = T/T_c$ is the reduced temperature, the critical temperature being $T_c = 369.80$ K according to Goodwin [130]. The value $\delta_H(T_b)$

$= 14.67 \text{ MPa}^{1/2}$ results. Gilmour et al. [98] reported the values $\Delta_v H(230 \text{ K})/\text{kcal mol}^{-1} = 4.48$ and $V(230 \text{ K})/\text{cm}^3 \text{mol}^{-1} = 75.3$, from which $\delta_H(T_b) = 14.94 \text{ MPa}^{1/2}$ is derived. Helpenstill and van Winkle [67] reported $\delta_H(T)/(\text{cal/cm}^3)^{1/2} = 6.92$ at 0°C and 6.54 at 25°C , that is, $\delta_H(273 \text{ K})/\text{MPa}^{1/2} = 14.15$ and $\delta_H(298 \text{ K})/\text{MPa}^{1/2} = 13.38$, the latter value being near that of LaPack et al. [28] at an unspecified temperature (presumably 25°C) of $13.6 \text{ MPa}^{1/2}$. Daura et al. [94] reported data obtained from their GROMOSC96 model, $\Delta_v H(T)/\text{kcal mol}^{-1} = 14.79$ and $\rho(T) = 493 \text{ kg m}^{-3}$ at $T = 298$ K, from which $\delta_H(298 \text{ K})/\text{MPa}^{1/2} = 12.30$. The value at the boiling point, $\delta_H(T_b) = 14.90 \text{ MPa}^{1/2}$, is selected here. Then temperature dependence of δ_H is shown in Table 3.

2.1.50. Octafluoropropane. Gilmour et al. [98] reported data for C_3F_8 at several temperatures from 230 to 237 K, from which the values at $T_b = 236.5$ K are readily derived, $\Delta_v H(T_b) = 4.70 \text{ kcal mol}^{-1}$ ($= 19.79 \text{ kJ mol}^{-1}$), $V(T_b) = 116.8 \text{ cm}^3 \text{mol}^{-1}$, and $\delta_H(T_b)/\text{MPa}^{1/2} = 12.28$. The computer simulations of Watkins and Jorgensen [99] agree with experimental values, yielding $\Delta_v H(T_b) = 4.73 \text{ kcal mol}^{-1}$ ($= 19.66 \text{ kJ mol}^{-1}$), $V(T_b) = 117.1 \text{ cm}^3 \text{mol}^{-1}$, and $\delta_H(T_b)/\text{MPa}^{1/2} = 12.26$. Sharafi and Boushehri [115] reported the following values: $T_b = 236.65$ K, $\rho(T_b) 1603 \text{ kg m}^{-3}$, and $\Delta_v H(T_b)/R = 2351.9$ K, from which $\delta_H(T_b) = 12.24 \text{ MPa}^{1/2}$ is derived. The mean value $\delta_H(T_b)/\text{MPa}^{1/2} = 12.26$ is selected here. Then temperature dependence of δ_H is shown in Table 3.

2.1.51. Ethyl Methyl Ether. The molar enthalpy of vaporization of $\text{CH}_3\text{OC}_2\text{H}_5$ at its boiling point of 7.35°C ($T_b = 280.5$ K) was reported by Ambrose et al. [131] as 25.1 kJ mol^{-1} . A slightly lower value, $5.91 \text{ kcal mol}^{-1}$, that is, $24.73 \text{ kJ mol}^{-1}$, was reported by Maass and Boomer [116]. These authors quoted Aronovich et al. [132] for the density $\rho(T_b) = 0.7205 \text{ g cm}^{-3}$, so that the solubility parameters resulting from the above two values of $\Delta_v H(T_b)$ are $\delta_H(T_b)/\text{MPa}^{1/2} = 16.52$ and 16.38 . The mean, 16.45 , is selected here as representative.

2.1.52. 1-Butene. Helpenstill and van Winkle [67] reported $\lambda(T)/(\text{cal/cm}^3)^{1/2} = 7.24$ at 0°C and 6.90 at 25°C and $\tau(T)/(\text{cal/cm}^3)^{1/2} = 1.43$ at 0°C and 1.32 at 25°C , where λ pertains to the dispersion aspect and τ to the polarity aspects ($\tau = 0$ for the saturated hydrocarbons). The total solubility parameter for $1\text{-C}_4\text{H}_8$ is $\delta_H(T) = (\lambda^2 + \tau^2)^{1/2}$, that is, $15.10 \text{ MPa}^{1/2}$ at 0°C and $14.37 \text{ MPa}^{1/2}$ at 25°C . Jorgensen et al. [93] reported $\Delta_v H(298 \text{ K})/\text{kcal mol}^{-1} = 4.87$ and $V(298 \text{ K})/\text{\AA}^3 \text{molecule}^{-1} = 158.2$, that is, $95.27 \text{ cm}^3 \text{mol}^{-1}$, resulting in $\delta_H(298 \text{ K})/\text{MPa}^{1/2} = 13.81$. Spyriouni et al. [133] reported results from molecular dynamics simulations over the temperature range 290 to 390 K, extrapolating to $T_b = 267.5$ K as $\Delta_v H(T_b)/\text{J mol}^{-1} = 20480$ and $\rho(T_b)/\text{g cm}^{-3} = 0.5738$, resulting in $\delta_H(T_b) = 13.66 \text{ MPa}^{1/2}$ and the temperature dependence is shown in Table 3. The Handbook [7] reports $T_b = 266.9$ K and $\Delta_v H(T_b)/\text{kJ mol}^{-1} = 22.07$ and with the extrapolated molar volumes from [67] $V(T_b) =$

$89.07 \text{ cm}^3 \text{ mol}^{-1}$ the resulting solubility parameter is $\delta_H(T_b = 266.9 \text{ K})/\text{MPa}^{1/2} = 14.93$, being selected here.

2.1.53. Cyclobutane. Only scant relevant data are available for $c\text{-C}_4\text{O}_8$, namely, from Helgeson et al. [128] $\Delta_v H(T_b)/\text{kcal mol}^{-1} = 5.78$ and $\rho(T_b)/\text{g cm}^{-3} = 0.732$, the boiling point being [7] -12.6°C , that is, $T_b = 260.6 \text{ K}$. The resulting $\delta_H(T_b) = 16.95 \text{ MPa}^{1/2}$. $\Delta_v H(T_b)/\text{kJ mol}^{-1} = 24.19$ in the Handbook [7] yields practically the same solubility parameter. The density in the Handbook pertaining to 25°C , $\rho(298)/\text{g cm}^{-3} = 0.6890$, and the molar volume $V(182.34 \text{ K}) = 69.62 \text{ cm}^3 \text{ mol}^{-1}$ from Martins et al. [134] are irrelevant here.

2.1.54. Octafluorocyclobutane. The computer simulations of Watkins and Jorgensen [99] do not agree very well with experimental values (translated from the engineering values of Martin [135] in psi and ft^3/lb), $\Delta_v H(T_b) = 4.69 \text{ kcal mol}^{-1}$ ($= 19.62 \text{ kJ mol}^{-1}$) and $\rho(T_b) = 1.753 \text{ g cm}^{-3}$, and there is also a misprint in their T_b : -40.20 instead of -4.20°C , the correct value being $T_b = 267.3 \text{ K}$. The experimental data yield $\delta_H(T_b) = 13.67 \text{ MPa}^{1/2}$, whereas the computed data yield $14.14 \text{ MPa}^{1/2}$, the former value being preferred.

2.1.55. *n*-Butane. Yosim and Owens [21] reported data from secondary sources $\Delta_v H(T_b)/\text{cal mol}^{-1} = 5352$ and $\rho(T_b)/\text{g cm}^{-3} = 0.601$ at $T_b = 272.7 \text{ K}$, from which $\delta_H(T_b)/\text{MPa}^{1/2} = 14.43$ is derived. Bradford and Thodos [66] reported the parameters of the expression (5), where $\delta_c = 2.259 (\text{cal}/\text{cm}^3)^{1/2}$, $k = 7.42$, $m = 0.446$, and $T_R = T/T_c$, $T_c = 425.14 \text{ K}$ from Kratzke et al. [136], with the value $\delta_H(T_b) = 14.24 \text{ MPa}^{1/2}$ resulting. Gilmour et al. [98] reported $\Delta_v H(T_b)/\text{kcal mol}^{-1} = 5.35$ and $V(T_b)/\text{cm}^3 \text{ mol}^{-1} = 96.4$ from which $\delta_H(T_b)/\text{MPa}^{1/2} = 14.45$ is derived. Helpenstill and van Winkle [67] reported $\delta_H(T)/(\text{cal}/\text{cm}^3)^{1/2} = 7.25$ at 0°C , and 6.954 at 25°C , and 6.77 at 45°C , extrapolating to $\delta_H(T_b)/\text{MPa}^{1/2} = 14.82$. Das et al. [137] reported the molar enthalpies and volumes of liquid and gaseous butane over the temperatures from T_b to T_c , from which the expression in Table 3 is derived and $\delta_H(T_b)/\text{MPa}^{1/2} = 14.43$ as from the previous authors. An appreciably smaller value, $\delta_H/\text{MPa}^{1/2} = 13.9$, at an unspecified temperature (presumably 298 K) was reported by LaPack et al. [28]. This value is near that, 13.75 , derived from the $\Delta_v H(298)$ and $\rho(298)$ obtained from GROMOSC96 model of Daura et al. [94]. The mean of the mutually agreeing values, $\delta_H(T_b)/\text{MPa}^{1/2} = 14.47$, is selected here.

2.1.56. *n*-Decafluorobutane. Brown and Mears [138] provided the required data for $n\text{-C}_4\text{F}_{10}$: $T_b = -2.00^\circ\text{C}$ ($T_b = 271.15 \text{ K}$), $\Delta_v H(T_b)/\text{kcal mol}^{-1} = 5.480$ ($= 22.93 \text{ kJ mol}^{-1}$), and the density interpolated in the reported data $\rho(T_b)/\text{g cm}^{-3} = 1.5925$, yielding $\delta_H(T_b)/\text{MPa}^{1/2} = 11.76$. The data provided by Gilmour et al. [98] lead to a similar value, $\delta_H(T_b)/\text{MPa}^{1/2} = 11.78$, whereas the simulation of Watkins and Jorgensen [99] yielded a slightly lower value, $\delta_H(T_b)/\text{MPa}^{1/2} = 11.69$. The mean of the two agreeing values is selected here, $11.77 \text{ MPa}^{1/2}$.

TABLE 1: Selected solubility parameters of liquefied inorganic gases at their boiling points.

Gas	T_b/K	$\delta_H/\text{MPa}^{1/2}$
He	4.22	1.22
Ne	27.07	10.01
Ar	87.30	14.21
Kr	119.9	15.24
Xe	165.0	16.1
Rn	211.5	17.1
H ₂	20.28	5.08
N ₂	77.36	11.95
O ₂	90.20	14.64
BF ₃	172.2	20.4
BCl ₃	285.8	16.1
CO	81.65	12.30
CO ₂	Sublimes	19.10(T_l)
COCl ₂	281.2	18.13
NF ₃	144.40	15.0
N ₂ O	184.7	20.58
NO	121.4	23.24
SF ₄	232.70	20.31
SF ₆	Sublimes	14.82(T_l)
B ₂ H ₆	180.6	14.19
SiH ₄	161.3	14.22
GeH ₄	185.05	14.97
SnH ₄	216.5	16.40
PH ₃	185.40	18.00
AsH ₃	210.65	18.27
SbH ₃	256.2	18.30
H ₂ S	213.6	20.72
H ₂ Se	231.90	20.97
H ₂ Te	270	20.8

2.1.57. Isobutane. Gilmour et al. [98] reported 2-methylpropane (isobutane) $\Delta_v H(T_b)/\text{kcal mol}^{-1} = 5.09$ and $V(T_b)/\text{cm}^3 \text{ mol}^{-1} = 97.8$ at $T_b = 261.4 \text{ K}$, from which $\delta_H(T_b)/\text{MPa}^{1/2} = 13.98$ is derived. Jorgensen et al. [93] reported similar values for $\Delta_v H(298)/\text{kcal mol}^{-1} = 4.57$ and $V(T_b)/\text{\AA}^3 \text{ molecule}^{-1} = 175.1$ from secondary sources as the previous authors resulting in $\delta_H(298)/\text{MPa}^{1/2} = 12.56$. Daura et al. [94] reported data obtained from their GROMOSC96 model, $\Delta_v H(T)/\text{kcal mol}^{-1} = 19.54$ and $\rho(T) = 551 \text{ kg m}^{-3}$ at $T = 298 \text{ K}$, from which $\delta_H(298 \text{ K})/\text{MPa}^{1/2} = 12.83$ results. The value at the boiling point, $\delta_H(T_b)/\text{MPa}^{1/2} = 13.98$, is selected here.

2.2. Results. The resulting selected $\delta_H(T_b)$ values are shown in Table 1 for inorganic liquefied gases and in Table 2 for organic ones (carbon compounds).

As the temperature is increased, the molar enthalpy of vaporization $\Delta_v H(T)$ diminishes towards its disappearance at the critical point. Over a temperature range near the normal boiling point T_b the function $\Delta_v H(T)$ is linear with the temperature. Also, as the temperature is increased,

TABLE 2: Selected solubility parameters of liquefied organic gases at their boiling points.

Gas	T_b/K	$\delta_H/MPa^{1/2}$
CH ₄	111.7	13.87
CH ₃ F	194.8	19.14
CH ₂ F ₂	221.6	21.02
CHF ₃	191.1	17.46
CF ₄	146.2	14.43
CH ₃ Cl	249.06	19.9
CH ₃ Br	276.70	19.9
HCHO	252	24.06
CH ₃ SH	279.1	20.26
C ₂ H ₂	Sublimes	18.9(T_l)
C ₂ H ₄	169.5	15.60
C ₂ H ₆	184.5	15.50
C ₂ H ₅ Cl	285.4	18.2
C ₂ F ₆	195.1	12.98
<i>c</i> -C ₂ H ₄ O	283.9	21.59
(CH ₃) ₂ O	248.4	17.65
C ₃ H ₆	225.4	15.36
<i>c</i> -C ₃ H ₆	240.3	17.7
C ₃ H ₈	231.1	14.90
C ₃ F ₈	236.5	12.26
CH ₃ OC ₂ H ₅	280.5	16.45
1-C ₄ H ₈	266.89	14.9
<i>c</i> -C ₄ H ₈	260.6	16.95
<i>c</i> -C ₄ F ₈	267.3	13.67
<i>n</i> -C ₄ H ₁₀	272.7	14.47
<i>n</i> -C ₄ F ₁₀	271.15	11.77
<i>i</i> -C ₄ H ₁₀	261.4	13.98

the density $\rho(T)$ diminishes and the molar volume $V(T)$ increases, both linearly over a temperature range near the normal boiling point T_b . Therefore, the solubility parameter $\delta_H(T) = [(\Delta_v H(T) - RT)/V(T)]^{0.5}$ necessarily diminishes as the temperature is increased. For several of the gaseous solutes for which there are data over a sufficient temperature range (excluding the noble gases) the decrease in $\delta_H(T)$ is linear with T with a slope of $-0.06 \pm 0.02 K^{-1}$ as is seen in Table 3. This slope may be used for the approximate estimation from the $\delta_H(T_b)$ values in Tables 1 and 2 of the applicable solubility parameter of the solute gases at the temperatures at which their solubility is needed.

3. Discussion

3.1. Trends in the Solubility Parameters. The following trends may be seen in the data of Tables 1 and 2, remembering that the normal boiling points may be considered as “corresponding temperatures” for the comparison of thermophysical data. $\delta_H(T_b)$ of the noble gases and of the hydrides of group IV and V elements increase with increasing molar masses of the gases. The opposite appears to be the case for homologous organic compounds. Polarity adds to the value arising from dispersion forces only, as, among others, Sistla et al. [36]

pointed out. Meyer et al. [100] calculated the contribution of the dispersion, polarity, and orientation to the cohesive energy, the dispersion part being 73 and 80% of the total for CH₃Cl and C₂H₅Cl, respectively, but did not obtain the solubility parameters.

3.2. Solubility Parameters Derived from Solubilities. In view of the concern with the solubility of gases in a variety of solvents, many authors have presented values of the solubility parameters of gases. Clever et al. [20] reported values of $\delta_H(T_b)/(\text{cal cm}^{-3})^{1/2}$ of the noble gases helium to xenon to one decimal digit that correspond well to the selected values in Table 1. These values, however, are larger (except for helium) than those derived from the relative solubilities in cyclohexane and perfluorocyclohexane. Vitovec and Fried [65] derived a value for $\delta_H(298 K)/(\text{cal cm}^{-3})^{1/2} = 6.75$ for acetylene, that is, as expected, smaller than the value at the triple point, 191.5 K, but agrees with the mean value derived from the solubility in benzene, toluene, and *p*-xylene, 6.86 $(\text{cal cm}^{-3})^{1/2}$. Prausnitz and Shair [27] reported values of $\delta_H/(\text{cal cm}^{-3})^{1/2}$ for Ar, Kr, Rn, N₂, O₂, CO, CO₂, CH₄, C₂H₄, and C₂H₆, suggested to be valid over a range of temperatures much larger than the boiling points. As expected, these values are smaller than $\delta_H(T_b)$. Similarly, Blanks and Prausnitz [64] reported values of $\delta_H(298 K)/(\text{cal cm}^{-3})^{1/2}$ from undisclosed sources for CH₄, C₂H₄, C₂H₆, C₃H₆, C₃H₈, and C₄H₁₀, shown in Table 4. Bradford and Thodos [66] provided the parameters for equation (5) for CH₄, C₂H₆, C₃H₈, and C₄H₁₀, from which solubility parameters at any temperature may be evaluated. The values at 298 K are shown in Table 4, except for methane, for which $T_c < 298 K$. Gilmour et al. [98] reported $\delta_H(T_b)/(\text{cal cm}^{-3})^{1/2}$ values for CF₄, C₂F₆, CH₄, C₂H₆, C₃H₈, and C₄H₁₀ that agree well with the values in Table 2. Helpenstill and van Winkle [67] reported the dispersion and polarity partial solubility parameters of hydrocarbons, which in the cases of C₃H₈ and C₄H₁₀ are only the dispersion ones, equaling $\delta_H/(\text{cal cm}^{-3})^{1/2}$ and shown in Table 4 for 298 K.

Lawson [62] reported values of $\delta_H(298 K)/(\text{cal cm}^{-3})^{1/2}$ for eight gases, obtained indirectly from their solubilities and are shown in Table 4. LaPack et al. [28] quoted previously reported values, as shown in Table 4. Sistla et al. [36] quoted the partial solubility parameters given by Hansen [2] for 298 K and the total (Hildebrand) solubility parameters shown in Table 4.

It should be remembered that at ambient conditions that pertain to Table 4 the solutes are gases. If the critical temperature is $T_c > 298 K$ they are liquid only under considerable pressure. Still, it has been tempting to take (1) to be valid at ambient conditions for these gaseous solutes, so that solubility parameters might be evaluated from the solubility data. In some cases the authors find lower solubility parameters of the solutes than from the relevant thermodynamic data at the boiling points of the liquefied gaseous solutes, for example, by Clever et al. [20] for noble gases and by Prausnitz and Shair [27] for these and other gases. In another case, in acetylene according to Vitovec and Fried [65], the nonideality of the gas had to be taken into account to obtain

TABLE 3: The temperature dependence of the solubility parameters of gaseous solutes, $\delta_H/\text{MPa}^{1/2} = A + B(T/K) + C(T/K)^2$, over the temperature range shown. The average uncertainties of A are $\pm 1.0\%$, of B are $\pm 2.6\%$, and of C are $\pm 5.0\%$.

Gas	Temperature range, T/K	A	B	C
Neon	25–40	8.036	0.3382	
Argon	84–87	21.95	−0.09028	−0.0098
Krypton	116–120	22.72	−0.0629	
Xenon	161–165	25.39	−0.05813	
Hydrogen	14–21	5.11	0.09611	
Oxygen	84–120	24.52	−0.1110	−0.004784
Carbon monoxide	68–81	19.13	−0.0837	
Carbon monoxide	80–110	21.47	−0.1121	
Carbon dioxide	217–290	−33.81	0.5243	
Phosgene	230–349	29.84	−0.0421	
Hydrogen sulfide	188–270	33.27	−0.05438	
Difluoromethane	200–280	49.56	−0.05606	
Trifluoromethane	180–260	30.11	−0.06632	
Tetrafluoromethane	120–200	22.79	−0.06299	
Ethylene	110–220	24.45	−0.05273	−0.001297
Ethylene oxide	235–375	35.44	−0.04894	
Cyclopropane	293–323	32.35	−0.05976	
Propane	210–230	23.85	−0.03870	
Octafluoropropane	200–237	20.24	−0.03359	
1-Butene	290–370	26.22	−0.04482	
Butane	280–350	25.86	−0.04133	

agreement between the solubility and thermodynamic values. Linford and Thornhill [24] related the solubilities of a variety of solvents in many solvents to the cohesive energy of the solute gases but did not use the solubility parameters. Lawson [62] used the solubility parameters of solute gases listed in Table 4 to calculate their solubilities in hydrocarbons and perfluorohydrocarbons. Lewis et al. [31] fitted the solubility of radon in selected perfluorocarbon solvents at 278 to 313 K by assigning it the value $8.42 \text{ cal}^{1/2} \text{ cm}^{-3/2}$ ($17.22 \text{ MPa}^{1/2}$).

Vetere [63] used solubility data of ten gases, H_2 , O_2 , N_2 , CH_4 , C_2H_4 , C_2H_6 , C_3H_8 , CO , CO_2 , and H_2S , in a variety of polar and nonpolar solvents and the NRTL (nonrandom two-liquid) model to obtain the (absolute) values of $\delta_{\text{HS}} - \delta_{\text{HG}}$. From these, with known values of the solvent δ_{HS} values, those for the solute gases could be estimated. The presented $\delta_{\text{HS}} - \delta_{\text{HG}}$ data pertained to a variety of temperatures for each solute gas, and it is difficult to obtain values for a definite temperature for all the solvents employed for a given gas. The mean values pertaining to $303 \pm 5 \text{ K}$ are listed in Table 4. Shamsipur et al. [139] dealt with the solubilities of gases in various solvents and reported “ δ_{H} ” values for the alkanes $\text{C}_n\text{H}_{2n+2}$ ($1 \leq n \leq 8$). When these are related to their known Hildebrand solubility parameters as solvents, the relationship $\delta_{\text{H}}/\text{MPa}^{1/2} = 7.65\delta_{\text{H}}^{0.2}$ results. When this relationship is applied to “ δ_{H} ” = 0.1402 for Ne this yields $\delta_{\text{H}} = 10.8 \text{ MPa}^{1/2}$. Note that for He the resulting value is too large, $10.6 \text{ MPa}^{1/2}$, so the approximate agreement for Ne should not be taken as valid.

As is seen in Table 4, the agreement between the entries for a given gas by diverse authors at a given temperature

near ambient is rather poor. This arises from the means used by the authors to calculate the values from solubilities, via (1) or equivalent expressions or based on other premises.

On the other hand, the miscibility of the liquefied gases among themselves should be directly related to their solubility parameters according to (1). Some data on the miscibility of gases were presented by Streng [69].

3.3. Correlations. The cohesive energies of permanent gases at their boiling points should be related to the attractive interactions of the particles. These, in turn, are related to the depths, ϵ , of the potential wells arising from the energetics of the collisions of the particles in the gas phase. A common measure of the energetics is the 12-6 Lennard-Jones relationship:

$$u = \epsilon \left[\left(\frac{r}{\sigma} \right)^{12} - \left(\frac{r}{\sigma} \right)^6 \right], \quad (6)$$

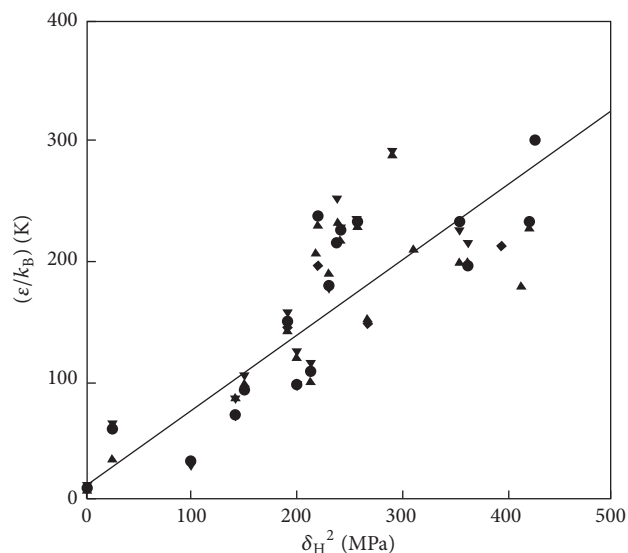
where r is the distance apart of the two colliding particles, σ is the distance of their centers at contact, and ϵ , reported in units of the Boltzmann constant in Kelvins, that is, $(\epsilon/k_{\text{B}})/\text{K}$, is the minimum of the interaction potential energy u . Indeed, the cohesive energy densities, $[\delta_{\text{H}}(T_{\text{b}})]^2$, are linearly related to the (ϵ/k_{B}) values of the gases for which values were found, see Figure 1. It should be noted that the (ϵ/k_{B}) reported by various authors, like De Ligny and Van der Veen [14], Teplyakov and Meares [13], Leites [12], and Churakov and Gottschalk [15],

TABLE 4: Literature values of solubility parameters of gases near ambient temperatures.

Gas	T/K	$\delta_H/\text{MPa}^{1/2}$	Ref.
He	298	1.0	[36]
Ar	273–333	10.9	[27, 28]
Kr	289–314	13.1	[27]
Rn	273–313	14.0	[27]
	298	17.2	[31]
H ₂	298	4.5	[62]
	298	5.1	[36]
N ₂	253–435	5.3	[27, 28]
	298	10.6	[62]
	298	11.9	[36]
	303	14.3	[63]
O ₂	273–333	8.2	[27, 28]
	298	11.7	[62]
	298	14.7	[36]
	303	10.2	[63]
CO	253–333	6.4	[27]
	298	11.9	[62]
	298	12.5	[36]
CO ₂	298	6.8	[62]
	298	12.3	[28]
	298	17.9	[36]
	313	22.5	[63]
NO	298	20.8	[36]
H ₂ S	298	20.7	[36]
	303	31.7	[63]
CH ₄	253–444	11.6	[27, 28]
	298	9.6	[64]
	298	12.7	[62]
	298	14.0	[36]
	303	14.7	[63]
CH ₃ Cl	298	19.8	[28]
C ₂ H ₂	298	13.8	[65]
	298	19.2	[36]
C ₂ H ₄	273–398	13.5	[27]
	298	11.3	[64]
	298	15.5	[36]
C ₂ H ₆	255–422	13.5	[27, 28]
	298	11.6	[64]
	298	8.0	[66]
	298	13.5	[62]
	298	15.6	[36]
	303	9.0	[63]
C ₃ H ₆	298	12.5	[64]
	298	12.7	[64]
	298	12.2	[66]
C ₃ H ₈	298	13.4	[67]
	298	13.6	[28, 62]
	412	11.7	[63]

TABLE 4: Continued.

Gas	T/K	$\delta_H/\text{MPa}^{1/2}$	Ref.
C ₄ H ₁₀	298	13.5	[64]
	298	13.5	[66]
	298	14.2	[67]
	298	13.9	[28]

FIGURE 1: The depth of the collision potential well of gas molecules, $(\epsilon/k_B)/K$, plotted against their cohesive density energy at the boiling point, δ_H^2/MPa . The symbols are for $(\epsilon/k_B)/K$ from [12] ●, from [13] ▼, from [14] ▲, and from [15] ◆.

among others, vary considerably as the figure shows. Still, a correlation

$$\left(\frac{\epsilon}{k_B}\right)/K = (10.4 \pm 10.7) + (0.65 \pm 0.05) [\delta_H(T_b)/\text{MPa}^{1/2}]^2 \quad (7)$$

with a correlation coefficient 0.9194 is found.

Another conceivable correlation of the solubility parameters of the liquefied gases would be with their surface tensions, σ . Data for the latter quantities are not plentiful but were found for a representative group of the gases treated here. Indeed, for the 17 liquefied gases for which surface tension data were found [16–19, 140] there is a linear relationship between the surface tension and the solubility parameter at the boiling point as follows:

$$\sigma(T_b)/\text{mN m}^{-2} = (-16.6 \pm 1.6) + (2.14 \pm 0.11) (\delta_H(T_b)/\text{MPa}^{1/2}) \quad (8)$$

with a correlation coefficient of 0.9797; see Figure 2. The value [18] for dimethyl ether is an outlier.

Koenhen and Smolders [141] reported the relationship between the dispersion solubility parameter and the index of

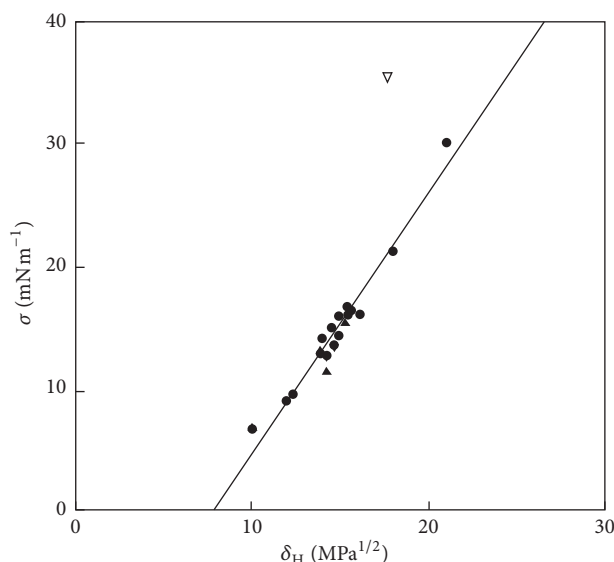


FIGURE 2: The surface tension of liquefied gases at their boiling points, $\sigma/\text{mN m}^{-2}$, plotted against their solubility parameters, $\delta_{\text{H}}/\text{MPa}^{1/2}$. The symbols are for the surface tension from [16, 17] ●, from [18] ▲, and [19] ▼, and for the outlier $(\text{CH}_3)_2\text{O}$, ▽ [18].

refraction, n_{D} , for many substances that are liquid at ambient temperatures, but not for those that are gases. The expression

$$\delta_{\text{H}}/(\text{cal cm}^{-3})^{1/2} = 9.55n_{\text{D}} - 5.55 \quad (9)$$

at an unspecified temperature (presumably 298 K) was found and may be applicable also for gaseous solutes.

4. Conclusions

The solubility parameters, $\delta_{\text{H}}(T_{\text{b}})$, of nonreactive permanent gases at their boiling points T_{b} (<290 K) including most inorganic gases (excluding reactive ones such as halogens and hydrogen halides) and organic ones up to butane are presented. They have been calculated from individually discussed values of their molar enthalpies of vaporization and densities obtained from the literature. Where available, the coefficients of the temperature dependence expression $\delta_{\text{H}}(T)$ are also tabulated. The $\delta_{\text{H}}(T_{\text{b}})$ values of representative inorganic gases increase with their molar masses but those of organic solutes (hydrocarbon) tend to diminish with increasing molar masses. The δ_{H} values generally diminish with increasing temperatures. Values of the solubility parameters reported in the literature that were derived from the solubilities of the gases in various solvents are inconsistent among various authors. The $\delta_{\text{H}}(T_{\text{b}})$ values correlate linearly with the attractive interaction energies of binary collisions of the gas molecules, the depths of the potential wells ε/k_{B} and with the surface tensions, $\sigma(T_{\text{b}})$, of the liquefied gases.

Competing Interests

The author declares that there are no competing interests regarding the publication of this paper.

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