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# POLYMER HANDBOOK

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FOURTH EDITION

Editors

J. BRANDRUP, E. H. IMMERGUT, and E. A. GRULKE

Associate Editors

A. ABE  
D. R. BLOCH



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# Contributors

- Abe, A.**  
Tokyo Institute of Polytechnics, Atsugi, Japan
- Allegra, G.**  
Dipartimento di Chimica del Politecnico, Milano, Italy
- Andreeva, L. N.**  
Institute of High Molecular Weight Compounds, Russian Academy of Sciences, St. Petersburg, Russian Federation
- Andrews, R. J.**  
Chemical and Materials Engineering Department, University of Kentucky, Lexington, Kentucky, USA
- Bai, F.**  
The Maurice Morton Institute of Polymer Science, Univeristy of Akron, Akron, USA
- Bareiss, R. E.**  
Editorial Office, Macromolecular Chemistry and Physics, Mainz, FR Germany
- Barrales-Rienda, J. M.**  
Instituto de Ciencia y Tecnología de Polímeros, Madrid, Spain
- Bello, A.**  
Instituto de Ciencia y Tecnología de Polímeros, Madrid, Spain
- Bello, P.**  
Instituto de Ciencia y Tecnología de Polímeros, Madrid, Spain
- Bloch, D. R.**  
Lakeshore Research, Racine, Wisconsin, USA
- Brandrup, J.**  
Wiesbaden, FR Germany
- Calhoun, B. H.**  
The Maurice Morton Institute of Polymers Science, University of Akron, Akron USA
- Casassa, E. F.**  
Department of Chemistry, Carneagie–Mellon University, Pittsburgh, Pennsylvania, USA
- Cheng, S. Z. D.**  
The Maurice Morton Institute of Polymer Science, University of Akron, Akron, Ohio, USA
- Chiu, F.-C.**  
The Maurice Morton Institute of Polymer Science, University of Akron, Akron, Ohio, USA
- Cho, J.**  
Polymer Science and Engineering Department, Dankook University, Seoul, South Korea
- Collins, E. A.**  
Avon Lake, Ohio, USA
- Daniels, C. A.**  
The Geon Company, Avon Lake, Ohio, USA
- DeLassus, P. T.**  
The Dow Chemical Company, Freeport, Texas, USA
- Dixon, K. W.**  
Akzo Nobel Chemicals, Inc., Dobbs Ferry, New York, USA
- Elias, H.-G.**  
Michigan Molecular Institute, Midland, Michigan, USA
- Fink, G.**  
Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, FR Germany
- Fink, H.-P.**  
Fraunhofer Institut für angewandte Polymerforschung, Teltow-Seehof, FR Germany
- Fouassier, J. P.**  
Laboratoire de Photochimie Générale, Ecole Nationale Supérieure de Chimie, Mulhouse, France
- Fu, Q.**  
The Maurice Morton Institute and Department of Polymer Science, University of Akron, Akron, Ohio, USA
- Furuta, I.**  
Japan Synthetic Rubber Company Ltd., Yokkaichi, Mie, Japan
- Ganster, J.**  
Fraunhofer Institute for Applied Polymer Research, Teltow-Seehof, Germany
- Greenley, R. Z.**  
Monsanto Corporation (retired), St. Louis, Missouri, USA
- Gulke, E. A.**  
Chemical and Materials Engineering, University of Kentucky, Lexington, Kentucky, USA
- Goh, S. H.**  
Department of Chemistry, National University of Singapore, Singapore
- Guzmán G. M.**  
Instituto de Ciencia y Tecnología de Polímeros, Madrid, Spain
- Hill, D. J. T.**  
Department of Chemistry, University of Queensland, St. Lucia, Australia
- Hiltner, A.**  
Department of Macromolecular Science, School of Engineering Case Western University, Cleveland, Ohio, USA
- Inomata, K.**  
Department of Polymer Chemistry, Tokyo Institute of Technology, Ookayama, Meguro-ku, Tokyo, Japan
- Iwama, M.**  
Japan Synthetic Rubber Company Ltd., Yokkaichi, Mie, Japan
- Jenkins, A. D.**  
School of Chemistry, Physics and Environmental Science, University of Sussex, Brighton, Sussex, UK
- Jenkins, J.**  
School of Chemistry, Physics and Environmental Science, University of Sussex, Brighton, Sussex, UK

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# Solubility Parameter Values

Eric A. Grulke

Chemical and Materials Engineering, University of Kentucky, Lexington, KY, USA

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## A. INTRODUCTION

Applications of solubility parameters include selecting compatible solvents for coating resins, predicting the swelling of cured elastomers by solvents, estimating solvent vapor pressure in polymer solutions for devolatilization and reaction systems (16), and predicting phase equilibria for polymer-polymer (107), polymer-binary (93), random copolymer (102), and multicomponent solvents (38, 98,108,109).

Cohesive energy density and solubility parameters are defined in the section on miscibility of solvents and polymers (Section B). In addition, the applicability of solubility parameters to thermodynamic calculations and their limitations are discussed. Section C contains methods for measuring, calculating and correlating solubility parameters of solvents and polymers. Section D contains

alphabetical listings of solubility parameters (Table 7), a list of solubility parameters in rank order (Table 8), a list of three-component solubility parameters of solvents (Table 9), and a list of solubility parameters of polymers (Table 10). With the exception of Table 7, solubility parameter values are reported in  $\text{MPa}^{1/2}$  units. The table showing solubility parameter value ranges for polymers (Table 3.4 in the third edition) has not been reproduced here.

## B. MISCIBILITY OF SOLVENTS AND POLYMERS

### 1. Cohesive Energy Density and the Solubility (Hildebrand) Parameter

Dissolution of an amorphous polymer in a solvent is governed by the free energy of mixing

$$\Delta G_m = \Delta H_m - T\Delta S_m \quad (\text{B1})$$

where  $\Delta G_m$  is the Gibbs free energy change on mixing,  $\Delta H_m$  is the enthalpy change on mixing,  $T$  the absolute temperature, and  $\Delta S_m$  is the entropy change on mixing. A negative value of the free energy change on mixing means that the mixing process will occur spontaneously. Otherwise, two or more phases result from the mixing process. Since the dissolution of a high molecular weight polymer is always connected with a small or modest increase in entropy, the enthalpy term (the sign and magnitude of  $\Delta H_m$ ) is the deciding factor in determining the sign of the Gibbs free energy change. Solubility parameters were developed to describe the enthalpy of mixing of simple liquids (nonpolar, nonassociating solvents), but have been extended to polar solvents and polymers.

Hildebrand and Scott (59) and Scatchard (101) proposed that

$$\Delta H_m = V \left( \left( \frac{\Delta E_1^v}{V_1} \right)^{1/2} - \left( \frac{\Delta E_2^v}{V_2} \right)^{1/2} \right)^2 \phi_1 \phi_2 \quad (\text{B2})$$

where  $V$  is the volume of the mixture,  $\Delta E_i^v$  the energy of vaporization of species  $i$ ,  $V_i$  the molar volume of species  $i$ , and  $\phi_i$  the volume fraction of  $i$  in the mixture.  $\Delta E_i^v$  is the energy change upon isothermal vaporization of the saturated liquid to the ideal gas state at infinite volume (94). The cohesive energy density (CED),  $\Delta E_i^v$ , is the energy of vaporization per  $\text{cm}^3$ . The solubility parameter has been defined as the square root of the cohesive energy density and describes the attractive strength between molecules of the material.

$$\delta_i = \left( \frac{\Delta E_i^v}{V_i} \right)^{1/2} \quad (\text{B3})$$

The dimensions of  $\delta_i$  are

$$\begin{aligned} (\text{cal/cm}^3)^{1/2} &= (4.187 \text{ J}/10^{-6} \text{ m}^3)^{1/2} \\ &= 2.046 \times 10^3 (\text{J/m}^3)^{1/2} = 2.046 \text{ MPa}^{1/2} \end{aligned} \quad (\text{B4})$$

The solubility parameter can be interpreted as the "internal pressure" of the solvent (9–11).  $\delta_i$  is called the Hildebrand parameter by some authors. Other researchers (13) prefer the term, "cohesion parameter", since it correlates with a large number of physical and chemical properties, and not just the miscibility of the components. The solubility parameter of a mixture is often taken as the sum of the products of the component solubility parameters with their volume fractions:

$$\delta_{\text{mixture}} = \sum_i \delta_i \phi_i \quad (\text{B5})$$

**Relation between  $\delta_i$  and  $\Delta H_m$**  Equation (B2) can be rewritten to give the heat of mixing per unit volume for a binary mixture:

$$\frac{\Delta H_m}{V} = (\delta_1 - \delta_2)^2 \phi_1 \phi_2 \quad (\text{B6})$$

Equation (B6) gives the heat of mixing of regular solutions in which the components mix with: (a) no volume change on mixing at constant pressure, (b) no reaction between the components, and (c) no complex formation or special associations (114). The heat of mixing must be smaller than the entropic term in Eq. (B1) for polymer-solvent miscibility ( $\Delta G_m \leq 0$ ). When  $\delta_1 = \delta_2$ , the free energy of mixing will always be less than zero for regular solutions and the components will be miscible in all proportions. In general, the solubility parameter difference,  $(\delta_1 - \delta_2)$  must be small for miscibility over the entire volume fraction range.

**Relation between  $\delta_i$  and  $\Delta H_i^v$**  The energy change on isothermal vaporization can be related to the enthalpy of vaporization:

$$\Delta E_i^v = \Delta H_i^v + \Delta H_i^\infty - RT + p^s V_i \quad (\text{B7})$$

where  $\Delta H_i^v$  is the enthalpy of vaporization at standard conditions,  $\Delta H_i^\infty$  the molar increase in enthalpy on isothermally expanding the saturated vapor to zero pressure,  $R$  the ideal gas constant, and  $p^s$  the saturation vapor pressure at temperature,  $T$ . At pressures below 1 atm, the  $\Delta H_i^\infty$  and  $p^s V_i$  terms are usually much less than the  $\Delta H_i^v$  and  $RT$  terms, and Eq. (B7) reduces to Eq. (B8):

$$\Delta E_i^v = \Delta H_i^v - RT \quad (\text{B8})$$

The solubility parameter of volatile materials (solvents for example) can be determined by measuring their enthalpy of vaporization or using a correlation for this quantity, and using Eq. (B9):

$$\delta_i = \left( \frac{\Delta H_i^v - RT}{V_i} \right)^{1/2} \quad (\text{B9})$$

Equation (B9) should be used at pressures near 1 atm. Near the critical point,  $\Delta H_i^v = 0$ , and Eq. (B8) incorrectly

predicts a negative value for the cohesive energy density while Eq. (B7) yields a small positive value.

**Dissolution of crystalline polymers** The free energy of mixing for crystalline polymers contains terms for the free energy of fusion for the crystalline volume fraction of the material. The free energy of fusion may contain terms that account for the loss of crystallite surface area and the mixing of amorphous material with oriented material. These terms would be added to Eq. (B1). The enthalpy of mixing could still be modeled using Eqs. (B2) or (B6). Some crystalline polymers obey the solubility parameter model at temperatures near their melting point,  $T > 0.9T_m$  (123). Solvent swelling experiments with crystalline polymers may fit Eq. (B1), particularly if the solvent is a poor one for the polymer and does not significantly dissolve crystalline regions.

### 2. Cohesive Energy Parameters for Polar Systems

The solubility parameter describes well the enthalpy change on mixing of nonpolar solvents but does not always give reliable results when extended to polar systems. The free energy change of mixing for polar systems is dominated by hydrogen-bonding forces between various groups in the solvent and polymer. Hydrogen-bonding forces are much stronger than van der Waals or dipole forces and often dominate the free energy of mixing. Complete miscibility is expected to occur if the solubility parameters are similar and the degree of hydrogen bonding (p: poor, m: moderate and s: strong) is similar between the components. Hydrocarbons, chlorinated hydrocarbons and nitrohydrocarbons are considered to be poor hydrogen-bonding solvents. Ketones, esters, and glycol monoethers give moderate hydrogen bonding. Alcohols, amines, acids, amides and aldehydes are strong hydrogen-bonding solvents. Table 7 classifies materials using these categories (21–24). Alternative classifications have been given by Lieberman (69), Gardon (41,85,86) and Dyck and Hoyer (32).

Other investigators have decomposed the Hildebrand parameter into several terms representing different contributions to the free energy of mixing. Hildebrand (59) used dispersive and polar solubility terms for solvents, with the complete parameter being given by

$$\delta^2 = \delta_d^2 + \delta_p^2 \quad (\text{B10})$$

where  $\delta_d$  is the dispersive term and  $\delta_p$  the polar term. The additional term improved agreement between  $\delta$  and experimental data. Prausnitz and coworkers accounted for polar bonding by including parameters for permanent dipole interactions and dispersion type interactions. This approach has been applied to polymer solutions (15) and complex formation (57). Crowley et al. (26,27) proposed a three-parameter system.

Hansen (49–53,56) and Hansen and Skaarup (54) assume that the cohesive energy arises from dispersive,

permanent dipole-dipole interactions and hydrogen bonding forces:

$$\delta^2 = \delta_d^2 + \delta_p^2 + \delta_h^2 \quad (\text{B11})$$

where  $\delta_h$  accounts for a variety of association bonds, including hydrogen bonds and permanent dipole-induced dipole (47). The values of these components for solvents were calculated from a large number of solubility data sets. Polymer solubility parameters can also be decomposed to a three-term set. The Hansen parameters give improved agreement with data but are still not completely accurate in predicting solutions thermodynamics for every system. Peiffer (172) has related dispersion, polar and induced solubility parameters to intermolecular forces and molecular size. The dispersive component increases with molecular size, while the polar component decreases with molecular size.

**Temperature effects** The solubility parameter decreases with temperature. The individual terms have varied dependence on temperature, namely (Ref. 55)

$$\begin{aligned} \frac{d\delta_d}{dT} &= -1.25 \times \alpha \times \delta_d \\ \frac{d\delta_p}{dT} &= -\frac{\delta_p \times \alpha}{2} \\ \frac{d\delta_h}{dT} &= -\delta_h \left( 1.22 \times 10^{-3} + \frac{\alpha}{2} \right) \end{aligned} \quad (\text{B12})$$

where  $\alpha (\text{K}^{-1})$  is the volumetric thermal expansion coefficient.

### 3. Relationship between Solubility Parameters and other Thermodynamic Parameters

Hildebrand and Hansen parameters can be calculated using other thermodynamic quantities. This section contains some of the relationships for binary systems. Extensions to multicomponent systems are described by Flory (37) and Olabisi et al. (89).

**Activity coefficients** Excess free energy calculations for regular solutions (93) can be used to relate solubility parameters and solvent activity coefficients:

$$RT \ln \gamma_1 = V_1 \phi_2^2 (\delta_1 - \delta_2)^2 \quad (\text{B13})$$

$$RT \ln \gamma_2 = V_2 \phi_1^2 (\delta_1 - \delta_2)^2 \quad (\text{B14})$$

where  $\gamma_i$  is the activity coefficient of component  $i$ . Equations (B13) and (B14) depend on the use of the geometric mean,  $\delta_{12} = (\delta_1 \times \delta_2)^{1/2}$ . Funk and Prausnitz (40) show that there are deviations from this rule for aromatic hydrocarbons.

**Molar excess free energy of mixing** The molar excess free energy of mixing for binary solutions is

$$\Delta G^E = \sum_i (\delta_{1-i} - \delta_{2-i})^2 \quad (\text{B15})$$

where  $\delta_{j-i}$  is the solubility term of group  $i$  for species  $j$ .



**Polymer-solvent interaction parameter** The polymer-solvent interaction parameter,  $\chi$ , is modeled as the sum of entropic and enthalpic components:

$$\chi = \chi_H + \chi_S \quad (\text{B16})$$

where  $\chi_H$  is the enthalpic component and  $\chi_S$  is the entropic component.  $\chi_S$  is usually taken to be a constant between 0.3 and 0.4 for nonpolar systems:  $\chi_S = 0.34$  is often used (15,104). The enthalpic component can be related to the Hildebrand parameters:

$$\chi_H = \frac{V_1}{RT}(\delta_1 - \delta_2)^2 \quad (\text{B17})$$

Substituting Eq. (B17) into Eq. (B16)

$$\chi = \frac{V_1}{RT}(\delta_1 - \delta_2)^2 + 0.34 \quad (\text{B18})$$

Equation (B18) permits only positive values of the interaction parameter. Since the Flory-Huggins criterion for complete solvent-polymer miscibility is  $\chi < 0.5$ , the enthalpic contribution must be small and the solubility parameters of the solvent and polymer must be similar (21). The molar volume of the solvent also affects miscibility and phase equilibria: a Hildebrand parameter needed for phase separation or miscibility cannot be specified without specifying  $V_1$ .

**Interchange energy density** Equation (B18) works well for nonpolar systems for which Eq. (B17) is a good description of the enthalpic component of the interaction parameter. The geometric mean assumption of regular solution theory is not appropriate for polar systems, and better models include an extra term describing the interchange energy density for the solvent-polymer pair. For example

$$\chi = \chi_S + \frac{V_1 A_{12}}{RT} \quad (\text{B19})$$

with

$$A_{12} = \delta_1^2 + \delta_2^2 - 2 \times l_{12} \delta_1 \delta_2 \quad (\text{B20})$$

where  $l_{12}$  characterizes the intermolecular forces between molecules (rather than using the geometric mean assumption). Equation (B20) allows the modeling of specific interactions between components 1 and 2. Mixed solvents can be treated as a single solvent by determining the solubility parameter of the solvent mixture, and then using this value in Eq. (B18). If both the solvents and the polymers interact, the description is more complicated. An alternative definition of  $A_{12}$  uses the two-component solubility parameter (Ref. 25)

$$A_{12} = (\delta_{1d} - \delta_{2d})^2 + (\delta_{1p} - \delta_{2p})^2 \quad (\text{B21})$$

The Hansen parameters may also be used to model  $A_{12}$ .

Several recent theories for polymer solution thermodynamics include entropic, enthalpic and free-volume contributions to the free energy of mixing. The free-volume contributions modify the entropic components, and have the opposite temperature dependence from the combinatorial term, helping to explain the lower critical solution temperature. Since Eq. (B18) assumes a constant value for the entropic component, it may not be valid over large temperature ranges. However, Eq. (B18) will predict the upper critical solution temperature, and, from this standpoint, is adequate for a number of phase equilibria applications near this condition.

The Lattice Fluid model (170) can be used to predict the solubilities of hydrocarbon and chlorinated hydrocarbons in nonpolar polymers. Three-dimensional solubility parameters can be used to provide an empirical correction to the geometric mean approximation (171). This correction predicts the solubility of polar and nonpolar solvents in polymers using only the pure component equation-of-state and solubility parameters.

**Guide to polymer-solvent miscibility** A region of solubility has been characterized by the distance between solvent and solute coordinates (Ref. 14)

$$R_{ij} = \left( 4(\delta_{1d} - \delta_{2d})^2 + (\delta_{1p} - \delta_{2p})^2 + (\delta_{1h} - \delta_{2h})^2 \right)^{1/2} \quad (\text{B22})$$

A more general definition of the region of solubility is

$$R_{ij} = \delta_1 - \delta_2 = (a(\delta_{1d} - \delta_{2d})^2 + b(\delta_{1p} - \delta_{2p})^2 + b(\delta_{1h} - \delta_{2h})^2)^{1/2} \quad (\text{B23})$$

where  $a$  and  $b$  are empirical weighing factors. If the distance between the solvent and the solute Hansen coordinate position exceeds  $R_{ij}$ , the two components are not soluble, or swelling is less than expected.  $R_{ij}$  reduces the need for three-dimensional plots. Some investigators have used two-dimensional plots for polar and hydrogen bonding terms, but the technique may be misleading for materials with large dispersion contributions. Barton (12) gives a number of models and contour map examples. As mentioned previously, Eqs. (B17)–(B19) suggest that the solvent molar volume can have a significant effect on miscibility.

Zeller (131) reviewed graphical three-dimensional solubility parameter estimation methods (12,14,49,55,172,173) as applied to solvent swelling of crosslinked elastomers. In general, the graphical method (Eqs. B22 and B23) does not account for the known influence of molar volume and crosslink density of solubility, and incorrectly assumes a linear relationship between the solubility parameter difference and solubility. An improved method used the Flory-Rehner equation to modify the interaction parameter for the effects of crosslink density (132).

**Guide to polymer-polymer miscibility** In many polymer-polymer systems, miscibility can be predicted by comparing the solubility parameters (139). The following table proposes miscibility guidelines. Polymer-polymer miscibility is enhanced when hydrogen bonding is present.

TABLE OF MISCIBILITY GUIDELINES<sup>a</sup>

| Intermolecular interaction | Polymer blend example                          | Critical value of the interaction parameter, $\chi_{crit}$ | Upper limit of the non-hydrogen bonded solubility parameter difference, $\Delta\delta$ (MPa <sup>1/2</sup> ) |
|----------------------------|------------------------------------------------|------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------|
| Dispersive forces only     | Polyisoprene-Poly(vinylethylene)               | <0.002                                                     | <0.02                                                                                                        |
| Dipole-dipole interactions | Poly(methyl methacrylate)-poly(ethylene oxide) | 0.002–0.001                                                | 0.2–1.0                                                                                                      |
| Weak hydrogen bonds        | Poly(vinyl chloride)-polycaprolactone          | 0.02–0.2                                                   | 1.0–2.0                                                                                                      |
| Moderate hydrogen bonds    | Poly(vinyl phenol)-poly(vinyl acetate)         | 0.2–1.0                                                    | 2.0–5.0                                                                                                      |
| Strong hydrogen bonds      | Poly(vinyl phenol)-poly(vinyl methyl ether)    | 1.0–1.5                                                    | 5.0–6.0                                                                                                      |

<sup>a</sup> Ref. 139.

## C. SOLUBILITY PARAMETER MEASUREMENTS, CALCULATIONS, AND CORRELATIONS

Solubility parameters can be determined by direct measurements, indirect calculations, or correlations with other physical parameters. The solubility parameters of solvents usually can be determined directly by measuring the energy of vaporization. The solubility parameters of polymers can only be determined indirectly and may be affected by variations in their chemical constitutions, i.e., the number of crosslinks and the distribution of chain branches or substitutive groups along the polymer backbone. The methods presented in this section can be used to develop correlations of solubility parameters with other physical properties for specific commercial polymer products or to estimate the solubility parameters of new polymers.

### 1. Solvents

**Calculation of the solubility term ( $\delta$ ) by relating the enthalpy of vaporization to the energy of vaporization** Equation (B8) can be used to calculate  $\Delta E_v^i$  when  $\Delta H_v^i$  is available. The molar volume of the solute is needed to complete the calculation of  $\delta$ , using Eq. (B3). This is the most direct and accurate method of determining the solubility parameter. However,  $\delta$ 's determined in this way may not give the best prediction of solution behavior. The solubility parameter values in Tables 7–9 reflect the solvent's behavior in a variety of systems.

**Correlations** Both the enthalpy of vaporization and the molar volume of a solvent can be estimated from

correlations. When  $\Delta H_v^i$  is known at the normal boiling point, it can be converted to the appropriate value at a second temperature using (126)

$$\frac{\Delta H_v^i(T_2)}{\Delta H_v^i(T_1)} = \left( \frac{T_c - T_2}{T_c - T_1} \right)^{0.38} \quad (\text{C1})$$

This corresponding state-type procedure gives estimates within 2% of experimental values over a wide range of temperatures (13). Hildebrand and Scott (59) proposed an empirical correlation between  $\Delta H_v^i$  at 25°C and the normal boiling point,  $T_b$ :

$$\Delta H_v^i(298K) = 0.2950 + 23.6 T_b + 0.020 T_b^2 \quad (\text{C2})$$

with enthalpy units of kcal/mol. Lawson (67) suggests different coefficients to include fluorocarbon liquids. The Clausius-Clapeyron equation can be applied if vapor pressure data are available. Eq. (C2) is reasonably accurate only for liquids that are not hydrogen bonded. The Hildebrand parameter calculated by Eq. (C2) should be adjusted as follows for different solvents (24): add 1.4 (cal/cm<sup>3</sup>)<sup>1/2</sup> for alcohols, add 0.6 (cal/cm<sup>3</sup>)<sup>1/2</sup> for esters, and add 0.5 (cal/cm<sup>3</sup>)<sup>1/2</sup> for ketones if the boiling point is less than 100°C. Jayasri and Yaseen (64) suggest adding 1.7 (cal/cm<sup>3</sup>)<sup>1/2</sup> for alcohols.

Solvent molar volumes are available or can be calculated by group molar volume methods at 25°C (35,163–165). The molar volume for solids at 25°C can be extrapolated from liquid state values (the liquid is assumed to be subcooled).

**Thermodynamic coefficients** The internal pressure,  $\pi$ , is defined as (Ref. 88)

$$\pi = \frac{\partial E}{\partial V} = T\beta - P \quad (\text{C3})$$

where  $\beta$  is the constant volume thermal pressure coefficient (the ratio of the coefficient of thermal expansion,  $\alpha$ , to the isothermal compressibility,  $\kappa$ ). Since the external pressure is usually small with respect to  $T\beta$ , the internal pressure is approximated by

$$\pi = T\beta = T \frac{\alpha}{\kappa} = T \left( \frac{\partial P}{\partial T} \right) \quad (\text{C4})$$

The Hildebrand parameter is the square root of the internal pressure. Eq. (C4) provides a method for scaling the Hildebrand parameter with temperature. This equation also provides a method for the direct estimation for  $\delta$  of polymers;  $\alpha$  and  $\kappa$  are measurable when  $\Delta H_v^i$  is not meaningful (B7). The thermal pressure coefficient (C4) can be evaluated from vapor-pressure data and is easier to apply than the Clausius-Clapeyron equation. For high pressure applications, such as phase equilibria in reverse osmosis membranes, the external pressure term in Eq. (C3) may not be negligible. Solubility parameters generally decrease with increasing pressure.

**van der Waals gas constant** Tables are available in many Handbooks for the van der Waals correction constants to the ideal gas law,  $a$  and  $b$ , where  $a$  has units of  $l^2/\text{atm}$ . For some liquids, these values may be at hand when other data are not available. They can be used to check Hildebrand parameter values obtained from other sources.

$$\delta = 1.2 \frac{\sqrt{a}}{V} \quad (C5)$$

The form of Eq. (C5) can be obtained by substituting the van der Waals equation of state into Eq. (C3).

**Critical pressure** The solubility parameter is related to the critical pressure,  $P_c$  of a substance through the empirical equation

$$\delta = 1.25 P_c^{1/2} \quad (C6)$$

where the critical pressure is expressed in atmospheres. Equation (C6) is not very accurate, but is simple to apply when critical pressure data are available.

**Surface tension** Michaels (83) has shown that the surface tension can be related to the cohesive energy density:

$$\frac{\Delta E_i^v}{V_i} = A \left( \frac{1}{V_i} \right)^{1/3} \gamma_L \quad (C7)$$

where  $\gamma_L$  is the surface tension and  $A$  is a constant. Koenhen and Smolders (65) correlated surface tension and two Hansen parameters:

$$\delta_d^2 + \delta_p^2 = 13.8 \left( \frac{1}{V_i} \right)^{1/3} \gamma_L \quad (C8)$$

$\delta_h$  is probably not related to the liquid-vapor interfacial energy as these interactions do not involve breaking hydrogen bonds. Eq. (C8) does not describe cyclic compound, acetonitrile, carboxylic acids, polyfunctional alcohols, and other polar compounds well. Hildebrand and Scott (59) have proposed a different equation, which has been discussed by Lee (68).

**Index of refraction** The dispersive Hansen parameter can be related to the index of refraction,  $n_D$  (65,105).

$$\delta_d = 9.55 n_D - 5.55 \quad (C9)$$

The interaction energy between nonpolar molecules should depend on polarizability (London dispersion forces) and, therefore, on the index of refraction.

**Dipole moment** Hansen and Skaarup (54) related the polar Hansen parameter to the dielectric constant,  $\epsilon$ , and the dipole moment,  $\mu$ :

$$\delta_p^2 = \frac{12108}{V^2} \frac{\epsilon - 1}{2\epsilon + n_D^2} (n_D^2 + 2) \mu^2 \quad (C10)$$

Beerbower and Dicky (14) proposed an empirical relationship:

$$\delta_p^2 = 9.5 \frac{\mu}{V_i^{1/2}} \quad (C11)$$

**Kauri butanol values** Proprietary hydrocarbon solvents are usually mixtures with boiling ranges and unknown molecular weights. Solubility parameter values may be estimated from Kauri butanol values (ASTM Method D1133-54T) using the equation

$$\delta = 6.3 + 0.03 KB \quad (C12)$$

## 2. Polymers

Hildebrand parameters cannot be calculated for polymers from heat of vaporization data because of their nonvolatility. Indirect methods are described below. The solubility parameter values in Table 10 may only be representative of a given polymer since variations in compositions can lead to changes in  $\delta$ .

### 2.1. Indirect Measurements

**Solvency testing (screening procedure)** The classic method for determining solubility parameter of a commercial polymer is solvency testing, or the solvency screening procedure. This technique compares polymer solubility in solvent groups with different hydrogen bonding characteristics (poor, moderate and strong). The midpoints of the polymer's solubility range may be used as single-valued quantities for some purposes, but may not agree with values determined by other methods (43). A gram or two of solid polymer is placed in a test tube and an approximate amount of a selected solvent is added such that the final solution would have about the correct solid content for the expected commercial use, e.g., 50% for alkyds, 20% for vinyls, etc. The exact amount is often unimportant, except for poor solvents. A typical phase diagram for binary polymer-solvent systems may show upper and lower critical solution temperatures. The one-phase region expands away from the UCST and LCST points, which often occur in the range of 20–80 wt.% polymer. The usual purpose of these experiments is to find good solvents for commercial product formulation, and this screening procedure will help identify such solvents. The mixture may be warmed and stirred to speed up solution, but it should be cooled and observed at room temperature. The resulting mixture should be a single phase, clear and free of gel particles or cloudiness. otherwise the polymer is judged insoluble. The solvents to be used are selected from Table 1.

This grouping of solvents has been selected so that the Hildebrand parameter values increase by reasonably constant steps within each hydrogen bonding class. The object of using these solvent spectra is to establish a solubility parameter range for a polymer rather than a single-valued number. This range has the advantage of showing the difference,  $(\delta_1 - \delta_2)^2$  (see Eqs. B13, B14 and

B18), which can be tolerated between the solubility values of the polymer and solvent for miscibility. Van Dyk et al. (120) have shown that the molar volume improves the correlation between solvency and the solubility parameters. A better measure of solubility might be the group,  $V_1(\delta_1 - \delta_2)^2$ .

In carrying out the procedure, it is convenient to select the first trials about 1/2 and 2/3 of the way down the column; for example, in the poorly hydrogen bonded group, toluene and nitroethane would be chosen. If the polymer is soluble in both, there is no need to try intermediate solvents because experience has shown that the polymer will be soluble in every case. The solvents at the end of the spectrum should be tried next. If the polymer is soluble in one but not both of the initial trials, the third trial should be half-way between the two. By successive choices, sets of two adjacent solvents will be found, one of which dissolves the polymer and one that does not. The parameter values of the solvents which do dissolve the polymer mark the ends of the range. The procedure is repeated for the other two hydrogen bonding classes.

**Osmotic pressure** Fedors (35) used the osmotic pressure of polymer solutions to determine solubility parameters.

**Swelling values** Another method for measuring the solubility parameter of polymers is to prepare a sparsely crosslinked sample and immerse it in a series of liquids of varying  $\delta$  (166,167). The crosslinked material will swell to varying degrees, with the maximum amount of swelling occurring when the solvent has the same Hildebrand parameter as the polymer. The amount of swelling can be measured by length, weight, or volume changes. By inference, the soluble, uncrosslinked materials has the same value. An example of a crosslinked sample is styrene polymerized with 1% divinyl benzene.

**Turbidity** Polymer can be precipitated from dilute solution by adding a non-solvent. The cloud point defines the onset of two phases. The enthalpic component of the interaction parameter,  $\chi_H$ , can be related to the solubility parameter difference between the solvent and the polymer (Eq. B17). Two different non-solvents are used: one having a solubility parameter above that of the solvent, and another having a solubility parameter below that of the solvent. The enthalpic components of the interaction parameter for each phase are equal at the cloud point, which can be used to measure the solubility parameter of the polymer (116). The two expressions for  $\chi_H$  are

$$\frac{V_{ml}(\delta_2 - \delta_{ml})^2}{RT} = \frac{V_{mh}(\delta_2 - \delta_{mh})^2}{RT} \quad (C13)$$

where  $V_{ml}$  and  $V_{mh}$  represent the molar volumes at the cloud points of the solvent-lower solubility parameter nonsolvent and solvent-higher solubility parameter nonsolvent, respectively.  $\delta_{ml}$  and  $\delta_{mh}$  are the solubility

parameters of the mixed solvents. The mixture properties are calculated using

$$\delta_m = \phi_1 \delta_1 + \phi_3 \delta_3 \quad (C14)$$

$$V_m = \frac{V_1 V_3}{\phi_1 V_3 + \phi_3 V_1} \quad (C15)$$

where the subscripts, 1 and 3, refer to the solvent and the nonsolvent. Eq. (C13) is simplified to determine the solubility parameter of the polymer:

$$\delta_2 = \frac{(\sqrt{V_{ml}} \delta_{ml} + \sqrt{V_{mh}} \delta_{mh})}{(\sqrt{V_{ml}} + \sqrt{V_{mh}})} \quad (C16)$$

The volume fraction of the nonsolvent at the cloud point is used to compute the solvent mixture solubility parameter and molar volume. Cloud point experiments are done for a series of solvents with the two nonsolvents, generating a set of points,  $(\delta_1, \delta_2)$ . The intersection of the line defined by this set of points with the line,  $\delta_1 = \delta_2$ , determines the polymer's solubility parameter.

**Specific volume** The specific volume of polymers varies with the solvent. Good solvents give higher values of the specific volume while poor solvents give lower values. A plot of the polymer specific volume as a function of solubility parameter gives a maximum value, which is taken to be the solubility parameter of the polymer. High precision density measurements at carefully controlled temperatures are needed for this method (168). The partial specific volume is defined as

$$\bar{V}_i = \left. \frac{\partial V}{\partial c_i} \right|_{T,p,i \neq j} \quad (C17)$$

The specific volume of a nonideal two-component system is

$$V_{\text{spec}} = \phi_1 \bar{V}_1 + \phi_2 \bar{V}_2 \quad (C18)$$

where  $\bar{V}_2$  is the rate of change in volume of the solution when a very small amount of polymer is added. As the solvent volume fraction goes to one, the partial molar volume of solvent is constant and Eq. (C18) becomes

$$V_{\text{spec}} = \bar{V}_{1(c_2=0)} + \phi_2 \bar{V}_2 \quad (C19)$$

The maximum of the polymer partial specific volume is estimated by fitting a quadratic to the data (Ref. 142):

$$\bar{V}_2 = \bar{V}_{2,\text{max}} - A(\delta_1 - \delta_2)^2 \quad (C20)$$

It is possible to estimate the polymer solubility parameter with only two reference solvents (168), but more reliable values are found by using a range of solvents.

**Intrinsic viscosity** A number of researchers have used intrinsic viscosity to estimate Hildebrand parameters (74).



Flory (37) related intrinsic viscosity to polymer molecular weight and the chain-expansion factor. The chain-expansion factor can, in turn, be related to the polymer-solvent interaction parameter using the Flory-Huggins theory. Maximum coil extension should occur in solvents near the polymer's solubility parameter. A variety of models can be used to relate the interaction parameter to Hildebrand parameters (19,80,115,167-169). These equations are quadratic (Eq. C21) or take the form of a gaussian curve (Eq. C22):

$$[\eta] = [\eta]_{\max} - A(\delta_1 - \delta_2)^2 \quad (\text{C21})$$

$$[\eta] = [\eta]_{\max} \exp(-A(\delta_1 - \delta_2)^2) \quad (\text{C22})$$

where  $[\eta]$  is the intrinsic viscosity,  $[\eta]_{\max}$  the maximum intrinsic viscosity, and  $A$  the constant. These researchers have shown that Eq. (C14) gives a good correlation between solvency and Hansen parameters for methacrylate polymers.

**Inverse phase gas chromatography** This method has been used by a number of investigators to measure infinite dilution weight fraction activity coefficients (6,29-31,63,71,72,84,90,91,113). These coefficients can be related to Hildebrand parameters by using a thermodynamic theory for polymer solutions, such as Flory-Huggins theory. The polymer is the stationary phase in a gas chromatography column. Both binary and multicomponent equilibria (46,99,100) can be studied using this method. Chromatographic techniques have the advantage of rapid measurement of thermodynamic values once the columns have been made. The solubility parameter can be related to the specific retention volume of the solvent on the column. Both  $V_i$  and  $\Delta H_i^v$  must be known at the temperature of the column. Molar volumes for the solvents can be determined by using literature density equations or generating equations from density data. Values for the enthalpy of vaporization can be determined at the experimental temperature (71).

The inverse phase gas chromatography method has the advantage of providing values for the infinite dilution solubility parameter,  $\delta_i^\infty$ , over a range of temperatures. This is particularly valuable for the prediction of phase equilibria at elevated temperatures. The value of  $\delta_i^\infty$  at 25°C can be estimated by using the expected temperature dependence for  $\chi$  (Eq. B18) of

$$\chi = \alpha + \frac{\beta}{T} \quad (\text{C23})$$

One potential problem with this technique is that  $\chi$  is known to be a function of concentration and the polymer Hildebrand parameter is determined at infinite dilution of solvent. For a number of binary systems, the change in  $\chi$  with solvent weight fraction is the largest as  $\omega \rightarrow 0$ . The concentration dependence of the interaction parameter can be modeled using methods given in the chapter on interaction parameters in this Handbook.

## 2.2. Correlation Methods

**Refractive index** Koenhen and Smolders (65) have predicted dispersive Hansen parameters from refractive index measurements of polymers. Wu (128) has suggested an effective cross-sectional area to relate the cohesive energy density and surface tension

$$\delta_d^2 = A \left( \frac{n_s}{V_{i,s}} \right)^{1/3} \gamma_s^d \quad (\text{C24})$$

where  $n_s$  is the number of atoms in a segment,  $V_{i,s}$  the molar volume of a segment, and  $\gamma_s^d$  the dispersion contribution to the free surface energy of the polymer.

**Dipole moment** Equation (C10) has been applied to polymers by Koenhen and Smolders (65). The dipole moments of polymers are between 70% and 90% of those of the corresponding monomer units.

**Hydrogen-bonding parameter** Hansen and Beerbower (55) compiled enthalpy data for hydrogen bonding groups. The following values are suggested:

| Group                  | Cohesive energy, $E_h$ , (kJ/mol) | Refs. |
|------------------------|-----------------------------------|-------|
| Alcohol                | 20.9                              | -     |
| Amide                  | 16.3                              | 83    |
| Ester                  | 5.2                               | 54    |
| Nitrile                | 2.1                               | 54    |
| Ether                  | 2.3                               | 54    |
| Monochloro substituent | 0.4                               | 54    |
| Phenylene ring         | 0.4                               | 54    |

The hydrogen-bonding parameter is given by

$$\delta_h^2 = \frac{E_h}{V_i} \quad (\text{C25})$$

**Group contribution methods** These methods have been used to estimate the solubility parameter (17,20,28,33,35, 58,60,61,96,112,121,122). van Krevelen (123), Fedors (35), and Barton (12) have reviewed these techniques and given tables of group values. The molar volume of solvents and polymers can also be estimated by group contribution techniques (108).

The sets of group constants of Small (112), Hoy (61) van Krevelen (121) and van Krevelen and Hoftyzer (122) seem to be most comprehensive. Table 2 gives the group molar attraction constants at 25°C. Small's values were derived from measurements of the heat of vaporization. Hoy's values were derived from vapor pressure measurements. The group contribution values of van Krevelen and Hoftyzer are based on cohesive energy data of polymers.

The group contribution techniques are based on the assumption that the contributions of different functional groups to the thermodynamic property are additive. The energy of vaporization of a solvent or polymer is

$$\Delta E_i^v = \sum_j n_j \Delta e_j \quad (\text{C26})$$

where  $\Delta e_j$  is the energy of vaporization contribution of group  $j$ , and  $n_j$  the number of groups of type  $j$  in the molecule. The solubility parameter is obtained by combining Eqs. (B3) and (C26):

$$\delta_i = \left( \frac{\Delta E_i^v}{V_i} \right)^{1/2} = \left( \frac{\sum_j n_j \Delta e_j}{V_i} \right)^{1/2} \quad (\text{C27})$$

Small (112) defined the molar attraction constant as

$$F_j = (\Delta E_{i,j}^v V_{i,j})^{1/2} \quad (\text{C28})$$

that can be used to calculate the solubility parameter by

$$\delta_i = \left( \frac{\Delta E_i^v V_i}{V_i^2} \right)^{1/2} = \frac{\sum_j F_j}{V_i} = \frac{\rho_i \sum_j F_j}{M_i} \quad (\text{C29})$$

where  $\rho_i$  is the polymer density and  $M_i$  is the polymer molecular weight.  $\delta_i$  can be evaluated for polymer repeating group by using group contribution calculations for the molar volume and the cohesive energy density or molar attraction constant. Table 2 gives sets of molar attraction constants and the energy of vaporization provided by several different authors. It is preferable to use parameters from only one set when determining the solubility parameter of a repeating unit. Table 3 gives the cohesive energy densities and group molar volumes determined by Fedors. This set may give less accurate estimates than those in Table 2, but it has value because it is more comprehensive and can be applied to more systems.

**Hansen parameters** The terms in Eq. (B11) can be estimated by group contribution methods. In general, the resulting factors are known less accurately than the group molar attraction constants or energy of vaporizations. The interaction of structural groups within molecules may not follow simple additive rules. However, the estimate of Hansen parameters can be very useful. Under the method of Hoftyzer and van Krevelen (Table 4), the terms are estimated as

$$\begin{aligned} \delta_d &= \frac{\sum F_{di}}{V} \\ \delta_p &= \frac{\sqrt{\sum F_{pi}^2}}{V} \\ \delta_h &= \frac{\sqrt{\sum E_{hi}}}{V} \end{aligned} \quad (\text{C30})$$

The dispersive Hansen parameter treats the molar attraction constants as additive. The polar Hansen parameters also are additive, unless more than one polar group is present. Methods for treating additional polar groups are given in

the last three rows of Table 4: additional polar groups do not add linearly to the polar Hansen term. The molar attraction constant is not applied to the hydrogen-bonding Hansen parameter. Rather, a hydrogen bonding energy,  $E_{hi}$ , is used.

Hoy (178-179) has an alternative group contribution method (Table 5). It includes a molar attraction function,  $F_{t,i}$  a polar component of this function,  $F_{p,i}$ , the molar volume of the solvent or polymer structural unit, the Lydersen correction for solvent non-ideality,  $\Delta_{T,i}$ , and a similar correction for polymer non-ideality,  $\Delta_{T,i}^{(P)}$ .

Bicerano (164) and Porter (165) have developed new group contribution techniques for a wide variety of polymer properties. These approaches consider how the different functional groups are connected in the molecule or in the polymeric repeating unit. Bicerano's method uses Fedor's (35) and van Krevelen's (123,163) group contribution values. Both references provide solubility parameter predictions of a number of polymers.

TABLE 1. SELECTED SOLVENTS FOR USE IN POLYMER SOLVENCY TESTING

| Solvent                    | $\delta$ (MPa <sup>1/2</sup> ) |
|----------------------------|--------------------------------|
| POORLY HYDROGEN BONDED     |                                |
| <i>n</i> -Pentane          | 14.3                           |
| <i>n</i> -Heptane          | 15.1                           |
| Methylcyclohexane          | 16.0                           |
| Solvesso 150               | 17.4                           |
| Toluene                    | 18.2                           |
| Tetrahydronaphthalene      | 19.4                           |
| <i>o</i> -Dichlorobenzene  | 20.5                           |
| 1-Bromonaphthalene         | 21.7                           |
| Nitroethane                | 22.7                           |
| Acetonitrile               | 24.1                           |
| Nitromethane               | 26.0                           |
| MODERATELY HYDROGEN BONDED |                                |
| Diethyl ether              | 15.2                           |
| Diisobutyl ketone          | 16.0                           |
| <i>n</i> -Butyl acetate    | 17.4                           |
| Methyl propionate          | 18.2                           |
| Dibutyl phthalate          | 19.0                           |
| Dioxane                    | 20.3                           |
| Dimethyl phthalate         | 21.9                           |
| 2,3-Butylene carbonate     | 24.8                           |
| Propylene carbonate        | 27.2                           |
| Ethylene carbonate         | 30.1                           |
| STRONGLY HYDROGEN BONDED   |                                |
| 2-Ethyl hexanol            | 19.4                           |
| Methyl isobutyl carbinol   | 20.5                           |
| 2-Ethyl butanol            | 21.5                           |
| <i>n</i> -Pentanol         | 22.3                           |
| <i>n</i> -Butanol          | 23.3                           |
| <i>n</i> -Propanol         | 24.3                           |
| Ethanol                    | 26.0                           |
| Methanol                   | 29.7                           |

TABLE 2. GROUP CONTRIBUTIONS TO COHESIVE ENERGY DENSITY

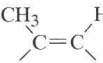
| Group                                                                               | F [MPa <sup>1/2</sup> cm <sup>3</sup> /mol] |                    | $\Delta E_i^v$ (J/mol) |                                 |
|-------------------------------------------------------------------------------------|---------------------------------------------|--------------------|------------------------|---------------------------------|
|                                                                                     | Small (112)                                 | van Krevelen (121) | Hoy (61)               | van Krevelen and Hoftyzer (163) |
| <b>2.1. CARBON-CONTAINING GROUPS</b>                                                |                                             |                    |                        |                                 |
| -CH <sub>3</sub>                                                                    | 437                                         | 420                | 303                    | 9630                            |
|    | 272                                         | 280                | 269                    | 4190                            |
|    | 57                                          | 140                | 176                    | 420                             |
|    | -190                                        | 0                  | 65                     | -5580                           |
| =CH <sub>2</sub>                                                                    | 388                                         | -                  | 259                    | -                               |
| =CH-                                                                                | 277                                         | 222                | 249                    | -                               |
| =C-                                                                                 | 39                                          | 82                 | 173                    | -                               |
| -CH=(aromatic)                                                                      | -                                           | -                  | 240                    | -                               |
| -C=(aromatic)                                                                       | -                                           | -                  | 201                    | -                               |
| -CH(CH <sub>3</sub> )-                                                              | 495                                         | 560                | (479)                  | (10060)                         |
| -C(CH <sub>3</sub> ) <sub>2</sub> -                                                 | 685                                         | 841                | (672)                  | (13700)                         |
| -CH=CH-                                                                             | 454                                         | 444                | 497                    | 10200                           |
| -C=CH-                                                                              | 265                                         | 304                | 421                    | 4860                            |
|    | (704)                                       | 724                | (725)                  | (14500)                         |
| H-C≡C-                                                                              | 583                                         | -                  | -                      | -                               |
| -C≡C-                                                                               | 454                                         | -                  | -                      | -                               |
| Cyclopentyl                                                                         | -                                           | 1380               | 1300                   | -                               |
| Cyclohexyl                                                                          | -                                           | 1660               | 1470                   | -                               |
| Phenyl                                                                              | 1500                                        | 1520               | (1400)                 | 31000                           |
| p-Phenylene                                                                         | 1350                                        | 1380               | (1440)                 | 25140                           |
| Naphthyl                                                                            | 2340                                        | -                  | -                      | -                               |
| <b>2.2. OXYGEN-CONTAINING GROUPS</b>                                                |                                             |                    |                        |                                 |
| -O-, ether                                                                          | 143                                         | 255                | 235                    | 6290                            |
| -O-, epoxide                                                                        | -                                           | -                  | 360                    | -                               |
| -OH                                                                                 | -                                           | 754                | 462                    | -                               |
| -OH, aromatic                                                                       | -                                           | -                  | 350                    | -                               |
| -(C=O)-                                                                             | 562                                         | 685                | 538                    | -                               |
| -(C=O)-O-                                                                           | 634                                         | 511                | 688                    | 13410                           |
| -(C=O)-OH                                                                           | -                                           | 651                | (998)                  | -                               |
| -O-(C=O)-O-                                                                         | -                                           | 767                | (904)                  | -                               |
| -(C=O)-O-(C=O)-                                                                     | -                                           | 767                | 1160                   | -                               |
| <b>2.3. NITROGEN-CONTAINING GROUPS</b>                                              |                                             |                    |                        |                                 |
| -NH <sub>2</sub>                                                                    | -                                           | -                  | 464                    | -                               |
| -NH-                                                                                | -                                           | -                  | 368                    | -                               |
|  | -                                           | -                  | 125                    | -                               |
| -CH-CN                                                                              | (896)                                       | 1120               | (901)                  | 25420                           |
| -CN                                                                                 | 839                                         | 982                | 725                    | 25000                           |
| -(C=O)-NH-                                                                          | -                                           | 1290               | (906)                  | 60760                           |
| -O-(C=O)-NH                                                                         | -                                           | 1480               | (1040)                 | -                               |
| -N=C=O                                                                              | -                                           | -                  | 734                    | -                               |
| <b>2.4. OTHER GROUPS</b>                                                            |                                             |                    |                        |                                 |
| -H                                                                                  | 164-205                                     | 140                | -103 (acidic dimer)    | -                               |
| -S-                                                                                 | 460                                         | 460                | 428                    | 8800                            |
| -SH                                                                                 | 644                                         | -                  | -                      | -                               |
| -F                                                                                  | (250)                                       | 164                | 84                     | 4470                            |
| -Cl (primary)                                                                       | 552                                         | 471                | 420                    | 12990                           |
| -Br (primary)                                                                       | 695                                         | 614                | 528                    | 15500                           |
| -I                                                                                  | 870                                         | -                  | -                      | -                               |
| -CF <sub>2</sub> -                                                                  | 307                                         | -                  | -                      | -                               |
| -CF <sub>3</sub>                                                                    | 561                                         | -                  | -                      | -                               |
| -O-N=O                                                                              | 900                                         | -                  | -                      | -                               |
| -NO <sub>2</sub>                                                                    | 900                                         | -                  | -                      | -                               |
| -PO <sub>4</sub>                                                                    | 1020                                        | -                  | -                      | -                               |
| -Si-                                                                                | -77                                         | -                  | -                      | -                               |

TABLE 2. cont'd

| Group                           | F [MPa <sup>1/2</sup> cm <sup>3</sup> /mol] |                    | $\Delta E_i^v$ (J/mol) |                                 |
|---------------------------------|---------------------------------------------|--------------------|------------------------|---------------------------------|
|                                 | Small (112)                                 | van Krevelen (121) | Hoy (61)               | van Krevelen and Hoftyzer (163) |
| <b>2.5. STRUCTURAL FEATURES</b> |                                             |                    |                        |                                 |
| Conjugation                     | 41-61                                       | -                  | 48                     | -                               |
| cis                             | -                                           | -                  | -15                    | -                               |
| trans                           | -                                           | -                  | -28                    | -                               |
| Ring, 4 member                  | -                                           | -                  | 159                    | -                               |
| 5 member                        | 215-235                                     | -                  | 43                     | -                               |
| 6 member                        | 194-215                                     | -                  | -48                    | -                               |
| Subscription, ortho             | -                                           | -                  | 20                     | -                               |
| meta                            | -                                           | -                  | 14                     | -                               |

TABLE 3. CONTRIBUTIONS TO *E*<sub>coh</sub> AND *V*<sup>a</sup>

| Group                                                                               | <i>E</i> <sub>coh</sub> (J/mol)            | <i>V</i> (cm <sup>3</sup> /mol) |
|-------------------------------------------------------------------------------------|--------------------------------------------|---------------------------------|
| -CH <sub>3</sub>                                                                    | 4710                                       | 33.5                            |
|  | 4940                                       | 16.1                            |
|  | 3430                                       | -1.0                            |
|  | 1470                                       | -19.2                           |
| =CH <sub>2</sub>                                                                    | 4310                                       | 28.5                            |
| =CH-                                                                                | 4310                                       | 13.5                            |
| =C-                                                                                 | 4310                                       | -5.5                            |
| H-C≡                                                                                | 3850                                       | 27.4                            |
| -C≡                                                                                 | 7070                                       | 6.5                             |
| Phenyl                                                                              | 31940                                      | 71.4                            |
| Phenylene: o, m, p                                                                  | 31940                                      | 52.4                            |
| Phenyl (trisubstituted)                                                             | 31940                                      | 33.4                            |
| (tetrasubstituted)                                                                  | 31940                                      | 14.4                            |
| (pentasubstituted)                                                                  | 31940                                      | -4.6                            |
| (hexasubstituted)                                                                   | 31940                                      | -23.6                           |
| Ring closure, 5 + atoms                                                             | 1050                                       | 16.0                            |
| 3 or 4 atoms                                                                        | 3140                                       | 18.0                            |
| Conjugation in ring for each double bond                                            | 1670                                       | -2.2                            |
| Halogen attached to carbon atom with double bond                                    | -20% of <i>E</i> <sub>coh</sub> of halogen | 4.0                             |
| -F                                                                                  | 4190                                       | 18.0                            |
| -F, disubstituted                                                                   | 3560                                       | 20.0                            |
| trisubstituted                                                                      | 2300                                       | 22.0                            |
| -CF <sub>2</sub> -, perfluoro compounds                                             | 4270                                       | 23.0                            |
| -CF <sub>3</sub> -, perfluoro compounds                                             | 4270                                       | 57.5                            |
| -Cl                                                                                 | 11550                                      | 24.0                            |
| -Cl, disubstituted                                                                  | 9630                                       | 26.0                            |
| trisubstituted                                                                      | 7530                                       | 27.3                            |
| -Br                                                                                 | 15490                                      | 30.0                            |
| -Br, disubstituted                                                                  | 12350                                      | 31.0                            |
| trisubstituted                                                                      | 10670                                      | 32.4                            |
| -I                                                                                  | 19050                                      | 31.5                            |
| -I, disubstituted                                                                   | 16740                                      | 33.5                            |
| trisubstituted                                                                      | 16330                                      | 37.0                            |
| -CN                                                                                 | 25530                                      | 24.0                            |
| -OH                                                                                 | 29800                                      | 10.0                            |
| -OH, disubstituted or adjacent C atoms                                              | 21850                                      | 13.0                            |
| -O-                                                                                 | 3350                                       | 3.8                             |
| -CHO, aldehyde                                                                      | 21350                                      | 22.3                            |
| -CO-                                                                                | 17370                                      | 10.8                            |
| -COOH                                                                               | 27630                                      | 28.5                            |
| -COO-                                                                               | 18000                                      | 18.0                            |
| -CO <sub>3</sub> -, carbonate                                                       | 17580                                      | 22.0                            |
| -C <sub>2</sub> O <sub>3</sub> -, anhydride                                         | 30560                                      | 30.0                            |

TABLE 3. cont'd

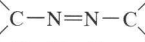
| Group                                                                                 | <i>E</i> <sub>coh</sub> (J/mol) | <i>V</i> (cm <sup>3</sup> /mol) |
|---------------------------------------------------------------------------------------|---------------------------------|---------------------------------|
| HCOO-, formate                                                                        | 18000                           | 32.5                            |
| -CO <sub>2</sub> CO <sub>2</sub> -, oxalate                                           | 26790                           | 37.3                            |
| -HCO <sub>3</sub>                                                                     | 12560                           | 18.0                            |
| -COF                                                                                  | 13400                           | 29.0                            |
| -COCl                                                                                 | 17580                           | 38.1                            |
| -COBr                                                                                 | 24150                           | 41.6                            |
| -COI                                                                                  | 29300                           | 48.7                            |
| -NH <sub>2</sub>                                                                      | 12560                           | 19.2                            |
| -NH-                                                                                  | 8370                            | 4.5                             |
|    | 4190                            | -9.0                            |
| -N=                                                                                   | 11720                           | 5.0                             |
| -NHNH <sub>2</sub>                                                                    | 21980                           | -                               |
| -N(NH <sub>2</sub> )-                                                                 | 16740                           | 16.0                            |
|  | 16740                           | 16.0                            |
| -N <sub>2</sub> , diazo                                                               | 8370                            | 23                              |
| -N=N-                                                                                 | 4190                            | -                               |
|  | 20090                           | -                               |
| -N=C=N-                                                                               | 11470                           | -                               |
| -N≡C                                                                                  | 18840                           | 23.1                            |
| -NF <sub>2</sub>                                                                      | 7660                            | 33.1                            |
| -NF-                                                                                  | 5070                            | 24.5                            |
| -CONH <sub>2</sub>                                                                    | 41860                           | 17.5                            |
| -CONH-                                                                                | 33490                           | 9.5                             |
|  | 29510                           | -7.7                            |
|  | 27630                           | 11.3                            |
| HCONH-                                                                                | 43950                           | 27.0                            |
| -NHCOO-                                                                               | 26370                           | 18.5                            |
| -NHCONH-                                                                              | 50230                           | -                               |
|  | 41860                           | -                               |
|  | 20930                           | -14.5                           |
| NH <sub>2</sub> COO-                                                                  | 37000                           | -                               |
| -NCO                                                                                  | 28460                           | 35.0                            |
| -ONH <sub>2</sub>                                                                     | 19050                           | 20.0                            |

TABLE 3. cont'd

| Group                        | $E_{coh}$ (J/mol) | $V$ (cm <sup>3</sup> /mol) |
|------------------------------|-------------------|----------------------------|
|                              | 25120             | 11.3                       |
| -CH=NOH                      | 25120             | 24.0                       |
| -NO <sub>2</sub> , aliphatic | 29300             | 24.0                       |
| -NO <sub>2</sub> , aromatic  | 15360             | 32.0                       |
| -NO <sub>3</sub>             | 20930             | 33.5                       |
| -NO <sub>2</sub> , nitrate   | 11720             | 33.5                       |
| -NHNO <sub>2</sub>           | 39770             | 28.7                       |
| -NNO-                        | 27210             | 10.0                       |
| -SH                          | 14440             | 28.0                       |
| -S-                          | 14150             | 12.0                       |
| -S <sub>2</sub> -            | 23860             | 23.0                       |
| -S <sub>3</sub> -            | 13400             | 47.2                       |
|                              | 39140             | -                          |
| SO <sub>3</sub>              | 18840             | 27.6                       |
| SO <sub>4</sub>              | 28460             | 31.6                       |
| -SO <sub>2</sub> Cl          | 37070             | 43.5                       |
| -SCN                         | 20090             | 37.0                       |
| -NCS                         | 25120             | 40.0                       |
| P                            | 9420              | -1.0                       |
| PO <sub>3</sub>              | 14230             | 22.7                       |
| PO <sub>4</sub>              | 20930             | 28.0                       |
| PO <sub>3</sub> -OH          | 31810             | 32.2                       |
| Si                           | 3390              | 0                          |
| SiO <sub>4</sub>             | 21770             | 20.0                       |
| B                            | 13810             | -2.0                       |
| BO <sub>3</sub>              | 0                 | 20.4                       |
| Al                           | 13810             | -2.0                       |
| Ga                           | 13810             | -2.0                       |
| In                           | 13810             | -2.0                       |
| Tl                           | 13810             | -2.0                       |
| Ge                           | 8080              | -1.5                       |
| Sn                           | 11300             | 1.5                        |
| Pb                           | 17160             | 2.5                        |
| As                           | 12980             | 7.0                        |
| Sb                           | 16330             | 8.9                        |
| Bi                           | 21350             | 9.5                        |
| Se                           | 17160             | 16.0                       |
| Te                           | 20090             | 17.4                       |
| Zn                           | 14480             | 2.5                        |
| Cd                           | 17790             | 6.5                        |
| Hg                           | 22810             | 7.5                        |

<sup>a</sup> Ref. 35.

TABLE 4. SOLUBILITY PARAMETER I: COMPONENT GROUP CONTRIBUTIONS<sup>a</sup>

| Structural Group        | $F_{di}$<br>(J <sup>1/2</sup> cm <sup>3/2</sup> /mol) | $F_{pi}$<br>(J <sup>1/2</sup> cm <sup>3/2</sup> /mol) | $E_{hi}$<br>(J/mol) |
|-------------------------|-------------------------------------------------------|-------------------------------------------------------|---------------------|
| -CH <sub>3</sub>        | 420                                                   | 0                                                     | 0                   |
|                         | 270                                                   | 0                                                     | 0                   |
|                         | 80                                                    | 0                                                     | 0                   |
|                         | -70                                                   | 0                                                     | 0                   |
| =CH <sub>2</sub>        | 400                                                   | 0                                                     | 0                   |
| =CH-                    | 200                                                   | 0                                                     | 0                   |
| =C-                     | 70                                                    | 0                                                     | 0                   |
|                         | 1620                                                  | 0                                                     | 0                   |
|                         | 1430                                                  | 110                                                   | 0                   |
|                         | 1270                                                  | 110                                                   | 0                   |
| -F                      | (220)                                                 | -                                                     | -                   |
| -Cl                     | 450                                                   | 550                                                   | 400                 |
| -Br                     | (550)                                                 | -                                                     | -                   |
| -CN                     | 430                                                   | 1100                                                  | 2500                |
| -OH                     | 210                                                   | 500                                                   | 20000               |
| -O-                     | 100                                                   | 400                                                   | 3000                |
| -COH                    | 470                                                   | 800                                                   | 4500                |
| -CO-                    | 290                                                   | 770                                                   | 2000                |
| -COOH                   | 530                                                   | 420                                                   | 10000               |
| -COO-                   | 390                                                   | 490                                                   | 7000                |
| HCOO-                   | 530                                                   | -                                                     | -                   |
| -NH <sub>2</sub>        | 280                                                   | -                                                     | 8400                |
| -NH-                    | 160                                                   | 210                                                   | 3100                |
|                         | 20                                                    | 800                                                   | 5000                |
| -NO <sub>2</sub>        | 500                                                   | 1070                                                  | 1500                |
| -S-                     | 440                                                   | -                                                     | -                   |
| =PO <sub>4</sub> -      | 740                                                   | 1890                                                  | 13000               |
| Ring                    | 190                                                   | -                                                     | -                   |
| One plane of symmetry   | -                                                     | 0.50 ×                                                | -                   |
| Two planes of symmetry  | -                                                     | 0.25 ×                                                | -                   |
| More planes of symmetry | -                                                     | 0 ×                                                   | 0 ×                 |

<sup>a</sup> Ref. 163.

TABLE 5. cont'd

| Group                        | $F_{ti}$<br>(J cm <sup>3</sup> ) <sup>1/2</sup> /mol) | $F_{pi}$<br>(J cm <sup>3</sup> ) <sup>1/2</sup> /mol) | $V_i$<br>(cm <sup>3</sup> /mol) | $\Delta T_i^*$ | $\Delta T_i^{(P)}$ |
|------------------------------|-------------------------------------------------------|-------------------------------------------------------|---------------------------------|----------------|--------------------|
| -CO-                         | 538                                                   | 525                                                   | 17.3                            | 0.040          | 0.040              |
| -COOH                        | 565                                                   | 415                                                   | 26.1                            | 0.039          | 0.039              |
| -COO-                        | 640                                                   | 528                                                   | 23.7                            | 0.047          | 0.050              |
| -CO-O-CO-                    | 1160                                                  | 1160                                                  | 41.0                            | 0.086          | 0.086              |
| -CN                          | 725                                                   | 725                                                   | 23.1                            | 0.060          | 0.054              |
| -N=C=O                       | 736                                                   | 8.2                                                   | 25.9                            | 0.054          | 0.054              |
| -N(HCO)-                     | 1020                                                  | 725                                                   | 35.8                            | 0.062          | 0.055              |
| -CONH <sub>2</sub>           | 1200                                                  | 900                                                   | 34.3                            | 0.071          | 0.084              |
| -CONH-                       | 1131                                                  | 895                                                   | 28.3                            | 0.054          | 0.073              |
| -OCONH-                      | 1265                                                  | 890                                                   | 34.8                            | 0.078          | 0.094              |
| -OH→H-bonded                 | 485                                                   | 485                                                   | 10.65                           | 0.082          | 0.034              |
| -OH, primary                 | 675                                                   | 675                                                   | 12.45                           | 0.082          | 0.049              |
| secondary                    | 591                                                   | 591                                                   | 12.45                           | 0.082          | 0.049              |
| tertiary                     | (500)                                                 | (500)                                                 | 12.45                           | 0.082          | 0.049              |
| phenolic                     | 350                                                   | 350                                                   | 12.45                           | 0.031          | 0.006              |
| -O-, ether                   | 235                                                   | 216                                                   | 6.45                            | 0.021          | 0.018              |
| acetal                       | 236                                                   | 102                                                   | 6.45                            | 0.018          | 0.018              |
| epoxide                      | 361                                                   | 156                                                   | 6.45                            | 0.027          | 0.027              |
| -NH <sub>2</sub>             | 464                                                   | 464                                                   | 17.0                            | 0.031          | 0.035              |
| -NH-                         | 368                                                   | 368                                                   | 11.0                            | 0.031          | 0.275              |
| -N-                          | 125                                                   | 125                                                   | 12.6                            | 0.014          | 0.009              |
| -S-                          | 428                                                   | 428                                                   | 18.0                            | 0.015          | 0.032              |
| -F                           | 845                                                   | 73.5                                                  | 11.2                            | 0.018          | 0.006              |
| -Cl, primary                 | 419.5                                                 | 307                                                   | 19.5                            | 0.017          | 0.031              |
| secondary                    | 426                                                   | 315                                                   | 19.5                            | 0.017          | 0.032              |
| aromatic                     | 330                                                   | 81.5                                                  | 19.5                            | 0.017          | 0.025              |
|                              | 705                                                   | 572                                                   | 39.0                            | 0.034          | 0.052              |
| -Br, aliphatic               | 528                                                   | 123                                                   | 25.3                            | 0.010          | 0.039              |
| aromatic                     | 422                                                   | 100                                                   | 25.3                            | 0.010          | 0.031              |
| Base value, B                | 277                                                   | -                                                     | -                               | -              | -                  |
| Ring, non-aromatic 4-member  | 159                                                   | 203                                                   | -                               | 0              | 0.012              |
| 5-member                     | 43                                                    | 85                                                    | -                               | 0              | 0.003              |
| 6-member                     | -48                                                   | 61                                                    | -                               | 0              | -0.0035            |
| 7-member                     | 92                                                    | 0                                                     | -                               | 0              | 0.007              |
| Conjugation, isomerism       | 47.5                                                  | -19.8                                                 | -                               | 0              | 0.0035             |
| cis                          | -14.6                                                 | -14.6                                                 | -                               | 0              | -0.001             |
| trans                        | -27.6                                                 | -27.6                                                 | -                               | 0              | -0.002             |
| Aromatic substitution, ortho | 20.2                                                  | -13.3                                                 | -                               | 0              | 0.0015             |
| meta                         | 13.5                                                  | -24.3                                                 | -                               | 0              | 0.001              |
| para                         | 83                                                    | -34.0                                                 | -                               | 0              | 0.006              |

<sup>a</sup> Ref. (178-179).

TABLE 5. SOLUBILITY PARAMETER II: COMPONENT GROUP CONTRIBUTIONS<sup>a</sup>

| Group                  | $F_{ti}$<br>(J cm <sup>3</sup> ) <sup>1/2</sup> /mol) | $F_{pi}$<br>(J cm <sup>3</sup> ) <sup>1/2</sup> /mol) | $V_i$<br>(cm <sup>3</sup> /mol) | $\Delta T_i^*$ | $\Delta T_i^{(P)}$ |
|------------------------|-------------------------------------------------------|-------------------------------------------------------|---------------------------------|----------------|--------------------|
| -CH <sub>3</sub>       | 303.5                                                 | 0                                                     | 21.55                           | 0.023          | 0.022              |
|                        | 269.0                                                 | 0                                                     | 15.55                           | 0.020          | 0.020              |
|                        | 176.0                                                 | 0                                                     | 9.56                            | 0.012          | 0.013              |
|                        | 65.5                                                  | 0                                                     | 3.56                            | 0              | 0.04               |
| =CH <sub>2</sub>       | 259                                                   | 67                                                    | 19.17                           | 0.018          | 0.019              |
| =CH-                   | 249                                                   | 59.5                                                  | 13.18                           | 0.018          | 0.0185             |
| =C-                    | 173                                                   | 63                                                    | 7.18                            | 0              | 0.013              |
| CH <sub>aromatic</sub> | 241                                                   | 62.5                                                  | 13.42                           | 0.011          | 0.018              |
| C <sub>aromatic</sub>  | 201                                                   | 65                                                    | 7.42                            | 0.011          | 0.015              |
| -HC=O                  | 600                                                   | 532                                                   | 23.3                            | 0.048          | 0.045              |

TABLE 6. EQUATIONS TO BE USED FOR HOY'S SYSTEM<sup>a</sup>

| Formulae                                          | Solvents                                                                                                                                                                                                  | Amorphous polymers                                                                                                       |
|---------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------|
| Additive molar functions                          | $F_t = \sum n_i F_{ti}$<br>$F_p = \sum n_i F_{pi}$<br>$V = \sum n_i V_i$<br>$\Delta T = \sum n_i \Delta T_i$                                                                                              | $F_t = \sum n_i F_{ti}$<br>$F_p = \sum n_i F_{pi}$<br>$V = \sum n_i V_i$<br>$\Delta T^{(P)} = \sum n_i \Delta T_i^{(P)}$ |
| Auxiliary equations                               | $\log \alpha = 3.39 \frac{T_b}{T_{cr}} - 0.1585 - \log V$<br>$T_b$ = boiling point, $T_{cr}$ = critical temp.<br>$\left(\frac{T_b}{T_{cr}}\right) = 0.567 + \Delta T - (\Delta T)^2$<br>Lydersen equation | $\frac{\alpha^{(P)}}{V} = \frac{777 \Delta T^{(P)}}{V}$<br>$\bar{n} = \frac{0.5}{\Delta T^{(P)}}$                        |
| Expressions for $\delta$ and $\delta$ -components | $\delta_t = \frac{F_t + B}{V}$ ; $B = 277$                                                                                                                                                                | $\delta_t = \frac{F_t + B}{V}$ ; $B = 277$                                                                               |



TABLE 6. cont'd

| Formulae                                                                        | Solvents | Amorphous polymers                                                                            |
|---------------------------------------------------------------------------------|----------|-----------------------------------------------------------------------------------------------|
| $\delta_p = \delta_t \left( \frac{1}{\alpha} \frac{F_p}{F_t + B} \right)^{1/2}$ |          | $\delta_p = \delta_t \left( \frac{1}{\alpha^{(P)}} \frac{F_p}{F_t + B/\bar{n}} \right)^{1/2}$ |
| $\delta_h = \delta_t \left( \frac{\alpha - 1}{\alpha} \right)^{1/2}$            |          | $\delta_h = \delta_t \left( \frac{\alpha^{(P)} - 1}{\alpha^{(P)}} \right)^{1/2}$              |
| $\delta_d = (\delta_t^2 - \delta_p^2 - \delta_h^2)^{1/2}$                       |          | $\delta_d = (\delta_t^2 - \delta_p^2 - \delta_h^2)^{1/2}$                                     |

<sup>a</sup> In the equations given here, *F<sub>t</sub>* is always combined with a Base value, *α* is the molecular aggregation number, and *n̄* the number of repeating units per polymer chain segment.

D. SOLUBILITY PARAMETER TABLES

TABLE 7. SOLUBILITY PARAMETERS OF SOLVENTS IN ALPHABETICAL ORDER

| Solvent                         | CAS number | Solubility parameter $\delta$ |                         | H-bonding group |
|---------------------------------|------------|-------------------------------|-------------------------|-----------------|
|                                 |            | (MPa <sup>1/2</sup> )         | (cal/cm) <sup>1/2</sup> |                 |
| Acetaldehyde                    | 75-07-0    | 21.1                          | 10.3                    | m               |
| Acetic acid                     | 64-19-7    | 20.7                          | 10.2                    | s               |
| Acetic anhydride                | 108-24-7   | 21.1                          | 10.3                    | s               |
| Acetone                         | 67-64-1    | 20.3                          | 9.9                     | m               |
| Acetonitrile                    | 75-07-8    | 24.3                          | 11.9                    | p               |
| Acetophenone                    | 98-86-2    | 21.7                          | 10.6                    | m               |
| Acetyl chloride                 | 75-36-5    | 19.4                          | 9.5                     | m               |
| Acetylmorpholine ( <i>N</i> )   | 1696-20-4  | 23.7                          | 11.6                    | m               |
| Acetylpiperidine ( <i>N</i> )   | 618-42-8   | 22.9                          | 11.2                    | s               |
| Acetylpyrrolidine ( <i>N</i> )  | 1072-83-9  | 23.3                          | 11.4                    | s               |
| Acrolein                        | 107-02-8   | 20.1                          | 9.8                     | s               |
| Acrylic acid                    | 79-10-7    | 24.6                          | 12.0                    | s               |
| Acrylonitrile                   | 107-13-1   | 21.5                          | 10.5                    | p               |
| Allyl acetate                   | 591-87-7   | 18.8                          | 9.2                     | m               |
| Allyl alcohol                   | 107-18-6   | 24.1                          | 11.8                    | s               |
| Allyl chloride                  | 107-05-1   | 18.0                          | 8.8                     | m               |
| Ammonia                         | 7664-41-7  | 33.4                          | 16.3                    | s               |
| Amyl acetate (iso)              | 625-16-1   | 16.0                          | 7.8                     | m               |
| (normal)                        | 628-63-7   | 17.4                          | 8.5                     | m               |
| (secondary)                     | 626-38-0   | 17.0                          | 8.3                     | m               |
| Amyl alcohol                    | 75-85-4    | 20.5                          | 10.0                    | s               |
| Amyl alcohol (normal)           | 71-41-0    | 22.3                          | 10.9                    | s               |
| Amylamine (normal)              | 110-58-7   | 17.8                          | 8.7                     | s               |
| Amyl bromide (1-bromopentane)   | 110-53-2   | 15.6                          | 7.6                     | m               |
| Amyl chloride (1-chloropentane) | 543-59-9   | 17.0                          | 8.3                     | m               |
| Amylene (2-methyl-2-butene)     | 513-35-9   | 14.1                          | 6.9                     | p               |
| Amyl ether (pentyl ether)       | 693-65-2   | 14.9                          | 7.3                     | m               |
| Amyl formate (iso)              | 110-45-2   | 16.4                          | 8.0                     | m               |
| (normal)                        | 638-49-3   | 17.2                          | 8.5                     | m               |
| Amyl iodide (1-iodopentane)     | 628-17-1   | 17.2                          | 8.4                     | m               |
| Anethole ( <i>para</i> )        | 4180-23-8  | 17.2                          | 8.4                     | m               |
| Aniline                         | 65-53-3    | 21.1                          | 10.3                    | s               |
| Anthracene                      | 120-12-7   | 20.3                          | 9.9                     | p               |
| Apco #18 solvent                |            | 15.3                          | 7.5                     | p               |
| Apco #140 solvent               |            | 14.9                          | 7.3                     | p               |
| Apco thinner                    |            | 16.0                          | 7.8                     | p               |
| Aroclor 1248                    | 12672-29-6 | 18.0                          | 8.8                     | p               |
| Benzaldehyde                    | 100-52-7   | 19.2                          | 9.4                     | m               |
| Benzene                         | 71-43-2    | 18.8                          | 9.2                     | p               |
| Benzonitrile                    | 100-47-0   | 17.2                          | 8.4                     | s               |
| Benzyl alcohol                  | 100-51-6   | 24.8                          | 12.1                    | p               |
| Bicyclohexyl                    | 92-51-3    | 17.4                          | 08.5                    | p               |
| Bromobenzene                    | 108-86-1   | 20.3                          | 09.9                    | p               |
| 1-Bromonaphthalene              | 90-11-9    | 21.7                          | 10.6                    | p               |
| Bromostyrene ( <i>ortho</i> )   | 2039-88-5  | 20.1                          | 9.8                     | p               |
| 1,3-Butadiene                   | 106-99-0   | 14.5                          | 7.1                     | p               |

TABLE 7. cont'd

| Solvent                                                        | CAS number | Solubility parameter $\delta$ |                         | H-bonding group |
|----------------------------------------------------------------|------------|-------------------------------|-------------------------|-----------------|
|                                                                |            | (MPa <sup>1/2</sup> )         | (cal/cm) <sup>1/2</sup> |                 |
| <i>n</i> -Butane                                               | 106-97-8   | 13.9                          | 6.8                     | p               |
| 1,3-Butanediol                                                 | 107-88-0   | 23.7                          | 11.6                    | s               |
| 1,4-Butanediol                                                 | 110-63-4   | 24.8                          | 12.1                    | s               |
| 2,3-Butanediol                                                 | 513-85-9   | 22.7                          | 11.1                    | s               |
| Butyl acetate (iso)                                            | 540-88-5   | 17.0                          | 8.3                     | m               |
| <i>n</i> -Butyl acetate                                        | 123-86-4   | 17.4                          | 8.5                     | m               |
| <i>sec</i> -Butyl acetate                                      | 105-46-4   | 16.8                          | 8.2                     | m               |
| Butyl acrylate (iso)                                           | 1663-39-4  | 17.4                          | 8.5                     | m               |
| <i>n</i> -Butyl acrylate                                       | 141-32-2   | 18.0                          | 8.8                     | m               |
| Butyl alcohol (iso) (2-methyl-1-propanol)                      | 78-83-1    | 21.5                          | 10.5                    | s               |
| <i>n</i> -Butyl alcohol (1-butanol)                            | 71-36-3    | 23.3                          | 11.4                    | s               |
| <i>sec</i> -Butyl alcohol (2-butanol)                          | 15892-23-6 | 22.1                          | 10.8                    | s               |
| <i>tert</i> -Butyl alcohol (2-methyl-2-propanol)               | 75-65-0    | 21.7                          | 10.6                    | s               |
| <i>n</i> -Butylamine                                           | 109-73-9   | 17.8                          | 8.7                     | s               |
| <i>n</i> -Butyl bromide (1-bromobutane)                        | 109-65-9   | 17.8                          | 8.7                     | m               |
| <i>sec</i> -Butyl bromide (2-bromobutane)                      | 78-76-2    | 17.2                          | 8.4                     | m               |
| Butyl (iso) butyrate (normal)                                  | 539-90-2   | 16.0                          | 7.8                     | m               |
| Butyl (normal) butyrate (normal)                               | 109-21-7   | 16.6                          | 8.1                     | m               |
| Butyl chloride (iso) (2-chloro-2-methylpropane)                | 507-20-0   | 16.6                          | 8.1                     | m               |
| Butylene-2,3 carbonate                                         | 4437-85-9  | 24.8                          | 12.1                    | m               |
| Butylene (iso) (2-methylpropene)                               | 115-11-7   | 13.7                          | 6.7                     | p               |
| Butyl ether                                                    | 142-96-1   | 16.0                          | 7.8                     | m               |
| Butyl formate (iso)                                            | 762-75-4   | 16.8                          | 8.2                     | m               |
| (normal)                                                       | 592-84-7   | 18.2                          | 8.9                     | m               |
| Butyl iodide (normal) (1-iodobutane)                           | 542-69-8   | 17.6                          | 8.6                     | m               |
| Butyl lactate (normal)                                         | 138-22-7   | 19.2                          | 9.4                     | m               |
| Butyl methacrylate                                             | 97-88-1    | 16.8                          | 8.2                     | m               |
| Butyl propionate                                               | 590-01-2   | 18.0                          | 8.8                     | m               |
| Butyl stearate                                                 | 123-95-5   | 15.3                          | 7.5                     | m               |
| Butyraldehyde                                                  | 123-72-8   | 18.4                          | 9.0                     | m               |
| Butyric acid (iso) (2-methylpropionic acid)                    | 79-31-2    | 21.1                          | 10.3                    | s               |
| (normal)                                                       | 107-92-6   | 21.5                          | 10.5                    | s               |
| Butyrolactone, $\gamma$                                        | 96-48-0    | 25.8                          | 12.6                    | m               |
| Butyronitrile (iso)                                            | 78-82-0    | 20.1                          | 9.8                     | p               |
| (normal)                                                       | 109-74-0   | 21.5                          | 10.5                    | p               |
| Caprolactam, $\epsilon$                                        | 105-60-2   | 26.0                          | 12.7                    | m               |
| Caprolactone, $\epsilon$                                       | 502-44-3   | 20.7                          | 10.1                    | m               |
| Capronitrile (heptyl cyanide)                                  | 124-12-9   | 19.2                          | 9.4                     | p               |
| Carbon disulfide                                               | 75-15-0    | 20.5                          | 10.0                    | p               |
| Carbon tetrachloride                                           | 56-23-5    | 17.6                          | 8.6                     | p               |
| Celanese solvent 601                                           |            | 18.8                          | 9.2                     | m               |
| Chloroacetone                                                  | 920-37-6   | 25.8                          | 12.6                    | p               |
| Chlorobenzene                                                  | 108-90-7   | 19.4                          | 9.5                     | p               |
| Chloroethyl acetate ( $\beta$ )                                | 542-58-5   | 19.8                          | 9.7                     | m               |
| Chloroform                                                     | 67-66-3    | 19.0                          | 9.3                     | p               |
| Chlorostyrene ( <i>ortho</i> or <i>para</i> )                  | 2039-87-4  | 19.4                          | 9.5                     | p               |
| Chlorotoluene ( <i>para</i> )                                  | 106-43-4   | 18.0                          | 8.8                     | p               |
| Cresol ( <i>meta</i> )                                         | 108-39-4   | 20.9                          | 10.2                    | s               |
| Cyclobutanedione                                               | 14406-53-3 | 22.5                          | 11.0                    | m               |
| Cyclohexane                                                    | 110-82-7   | 16.8                          | 8.2                     | p               |
| Cyclohexanol                                                   | 108-93-0   | 23.3                          | 11.4                    | s               |
| Cyclohexanone                                                  | 108-94-1   | 20.3                          | 9.9                     | m               |
| Cyclopentane                                                   | 287-92-3   | 17.8                          | 8.7                     | p               |
| Cyclopentanone                                                 | 120-92-3   | 21.3                          | 10.4                    | m               |
| Cymene ( <i>para</i> ) (2-isopropyl toluene)                   | 99-87-6    | 16.8                          | 8.2                     | p               |
| Decahydronaphthalene ( <i>cis</i> and <i>trans</i> ) (Decalin) | 91-17-8    | 18.0                          | 8.8                     | p               |
| Decane (normal)                                                | 124-18-5   | 13.5                          | 6.6                     | p               |
| Decyl acrylate (iso)                                           | 2156-96-9  | 16.8                          | 8.2                     | m               |
| Diacetone alcohol (4-hydroxy-4-methyl-2-pentanone)             | 123-42-2   | 18.8                          | 9.2                     | m               |
| Diacetone alcohol methyl ether (Pentoxone)                     | 107-70-0   | 16.8                          | 8.2                     | m               |
| Diamylpiperazine ( <i>N,N</i> )                                | 18940-57-3 | 28.0                          | 13.7                    | m               |
| Diamyl phthalate                                               | 131-18-0   | 18.6                          | 9.1                     | m               |
| Dibenzyl ether                                                 | 103-50-4   | 19.2                          | 9.4                     | m               |

TABLE 7. cont'd

| Solvent                                             | CAS number | Solubility parameter $\delta$ |                         | H-bonding group |
|-----------------------------------------------------|------------|-------------------------------|-------------------------|-----------------|
|                                                     |            | (MPa <sup>1/2</sup> )         | (cal/cm) <sup>1/2</sup> |                 |
| Dibromoethane-1,2                                   | 106-93-4   | 21.3                          | 10.4                    | p               |
| Dibromoethylene-1,2 ( <i>cis</i> and <i>trans</i> ) | 540-49-8   | 20.7                          | 10.1                    | p               |
| Dibutoxyethyl phthalate (Kronisol)                  | 117-83-9   | 16.4                          | 8.0                     | m               |
| Dibutylamine                                        | 111-92-2   | 16.6                          | 8.1                     | m               |
| Dibutyl fumarate                                    | 105-75-9   | 18.4                          | 9.0                     | m               |
| Dibutyl maleate                                     | 105-76-0   | 18.4                          | 9.0                     | m               |
| Dibutyl phenyl phosphate                            | 2528-36-1  | 17.8                          | 8.7                     | m               |
| Dibutyl phthalate                                   | 84-74-2    | 19.0                          | 9.3                     | m               |
| Dibutyl sebacate                                    | 109-43-3   | 18.0                          | 9.2                     | m               |
| Dichloroacetic acid                                 | 79-43-6    | 22.5                          | 11.0                    | s               |
| Dichlorobenzene ( <i>ortho</i> )                    | 95-50-1    | 20.5                          | 10.0                    | p               |
| Dichlorodifluoromethane (Freon 12)                  | 75-71-8    | 11.3                          | 5.5                     | p               |
| Dichloroethyl ether                                 | 623-46-1   | 20.1                          | 9.8                     | m               |
| Dichloroethylene, <i>cis</i> -1,2                   | 156-59-2   | 18.6                          | 9.1                     | m               |
| <i>trans</i> -1,2                                   | 156-60-5   | 18.4                          | 9.0                     | m               |
| Dichlorofluoromethane (Freon 21)                    | 75-43-4    | 17.0                          | 8.3                     | p               |
| Dichloropropane-1,2                                 | 78-87-5    | 18.4                          | 9.0                     | p               |
| Dichloropropane-2,2                                 | 594-20-7   | 16.8                          | 8.2                     | p               |
| Diethylacetamide ( <i>N,N</i> )                     | 685-91-6   | 20.3                          | 9.9                     | m               |
| Diethylamine                                        | 109-89-7   | 16.4                          | 8.0                     | m               |
| Diethyl carbonate                                   | 105-58-8   | 18.0                          | 8.8                     | m               |
| Diethylene glycol                                   | 111-46-6   | 24.8                          | 12.1                    | s               |
| Diethylene glycol monobutyl ether (normal)          | 112-34-5   | 19.4                          | 9.5                     | m               |
| Diethylene glycol monobutyl ether                   | 112-34-5   | 20.9                          | 10.2                    | m               |
| Diethylene glycol monobutyl ether acetate           | 124-17-4   | 17.4                          | 8.5                     | m               |
| Diethylene glycol monolaurate                       | 141-20-8   | 17.8                          | 8.7                     | m               |
| Diethyl ether                                       | 60-29-7    | 15.1                          | 7.4                     | m               |
| Diethylformamide ( <i>N,N</i> )                     | 617-84-5   | 21.7                          | 10.6                    | m               |
| Diethyl ketone                                      | 96-22-0    | 18.0                          | 8.8                     | m               |
| Diethyl maleate                                     | 141-05-9   | 20.3                          | 9.9                     | m               |
| Diethyl oxalate                                     | 95-92-1    | 17.6                          | 8.6                     | m               |
| Diethyl phthalate                                   | 84-66-2    | 20.5                          | 10.0                    | m               |
| Diethyl-2,2-propanediol-1,2 (heptylene glycol)      | 115-76-4   | 20.3                          | 9.9                     | m               |
| Diethyl sulfone                                     | 597-35-3   | 25.4                          | 12.4                    | m               |
| Difluorotetrachloroethane (Freon 112)               | 76-11-9    | 16.0                          | 7.8                     | p               |
| Diformylpiperazine ( <i>N,N</i> )                   | 4164-39-0  | 31.5                          | 15.4                    | m               |
| Dihexyl ether                                       | 112-58-3   | 16.4                          | 8.0                     | m               |
| Di- <i>n</i> -hexyl phthalate                       | 108-83-8   | 18.2                          | 8.9                     | m               |
| Diisobutylene                                       | 107-39-1   | 15.8                          | 7.7                     | m               |
| Diisobutyl ketone                                   | 108-83-8   | 16.0                          | 7.8                     | m               |
| Diisodecyl phthalate                                | 26761-40-0 | 14.7                          | 7.2                     | m               |
| Diisopropyl ether                                   | 108-20-3   | 14.1                          | 6.9                     | m               |
| Diisopropyl ketone                                  | 565-80-0   | 16.4                          | 8.0                     | m               |
| Dimethylacetamide ( <i>N,N</i> )                    | 127-19-5   | 22.1                          | 10.8                    | m               |
| Dimethylaniline                                     | 121-69-7   | 19.8                          | 9.7                     | m               |
| Dimethyl-2,2-butanediol-1,2 (isobutylene glycol)    | 558-43-0   | 22.9                          | 11.2                    | s               |
| Dimethyl-2,2-butanediol-1,3                         | 76-09-3    | 20.5                          | 10.0                    | s               |
| Dimethyl carbonate                                  | 616-38-6   | 20.3                          | 9.9                     | m               |
| Dimethyl ether                                      | 115-10-6   | 18.0                          | 8.8                     | m               |
| Dimethylformamide ( <i>N,N</i> )                    | 68-12-2    | 24.8                          | 12.1                    | m               |
| Dimethyl malonate                                   | 108-59-8   | 22.5                          | 11.0                    | m               |
| Dimethylnitroamine ( <i>N,N</i> )                   | 62-75-9    | 26.8                          | 13.1                    | m               |
| Dimethyl oxalate                                    | 553-90-2   | 22.5                          | 11.0                    | m               |
| Dimethyl phosphite                                  | 868-85-9   | 25.6                          | 12.5                    | m               |
| Dimethyl phthalate                                  | 131-11-3   | 21.9                          | 10.7                    | m               |
| Dimethyl siloxane                                   | 9016-00-6  | 10.0-12.1                     | 4.9-5.9                 | m               |
| Dimethyl sulfide                                    | 75-18-3    | 19.2                          | 9.4                     | m               |
| Dimethyl sulfoxide                                  | 67-68-5    | 29.7                          | 14.5                    | m               |
| Dimethyltetramethylene sulfone                      | 1003-78-7  | 24.6                          | 12.0                    | m               |
| Diocetyl adipate                                    | 103-23-1   | 17.8                          | 8.7                     | m               |
| Diocetyl phthalate                                  | 117-81-7   | 24.8                          | 12.1                    | m               |
| Diocetyl sebacate                                   | 1222-62-3  | 17.8                          | 8.7                     | m               |
| Dioxane-1,4                                         | 123-91-1   | 16.2                          | 7.9                     | m               |

TABLE 7. cont'd

| Solvent                                                       | CAS number | Solubility parameter $\delta$ |                         | H-bonding group |
|---------------------------------------------------------------|------------|-------------------------------|-------------------------|-----------------|
|                                                               |            | (MPa <sup>1/2</sup> )         | (cal/cm) <sup>1/2</sup> |                 |
| Dioxolane-1,3                                                 | 646-06-0   | 17.6                          | 8.6                     | m               |
| Dipentene                                                     | 138-86-3   | 20.5                          | 10.0                    | m               |
| Diphenyl ether                                                | 101-84-8   | 20.9                          | 10.2                    | m               |
| Diphenyl 2-ethylhexyl phosphate                               | 1241-94-7  | 17.4                          | 8.5                     | p               |
| Dipropylene glycol                                            | 110-98-5   | 20.7                          | 10.1                    | m               |
| Dipropylene glycol monomethyl ether                           | 34590-94-8 | 17.6                          | 8.6                     | m               |
| Dipropyl phthalate                                            | 131-16-8   | 20.5                          | 10.0                    | s               |
| Dipropyl sulfone                                              | 598-03-8   | 23.1                          | 11.3                    | m               |
| Dodecane                                                      | 112-40-3   | 16.2                          | 7.9                     | p               |
| Dodecanol-1                                                   | 112-53-8   | 20-21                         | 9.8                     | s               |
| Epichlorohydrin                                               | 106-89-8   | 22.5                          | 11.0                    | s               |
| Ethane                                                        | 74-84-0    | 12.3                          | 6.0                     | p               |
| Ethylacetamide ( <i>N</i> )                                   | 625-50-3   | 25.2                          | 12.3                    | s               |
| Ethyl acetate                                                 | 141-78-6   | 18.6                          | 9.1                     | m               |
| Ethyl acrylate                                                | 140-88-5   | 17.6                          | 8.6                     | m               |
| Ethyl alcohol                                                 | 64-17-5    | 26.0                          | 12.7                    | s               |
| Ethylamine                                                    | 75-04-7    | 20.5                          | 10.0                    | s               |
| Ethyl amyl ketone (3-octanone)                                | 106-68-3   | 16.8                          | 8.2                     | m               |
| Ethylbenzene                                                  | 100-41-4   | 18.0                          | 8.8                     | p               |
| Ethyl benzoate                                                | 93-89-0    | 16.8                          | 8.2                     | m               |
| Ethyl bromide (bromoethane)                                   | 74-96-4    | 19.6                          | 9.6                     | m               |
| Ethyl-2-butanol-1                                             | 97-95-0    | 21.5                          | 10.5                    | s               |
| Ethyl <i>n</i> -butyrate                                      | 105-54-4   | 17.4                          | 8.5                     | m               |
| Ethyl caprylate                                               | 106-32-1   | 14.9                          | 7.3                     | m               |
| Ethyl chloride                                                | 75-00-3    | 18.8                          | 9.2                     | m               |
| Ethyl cyanoacetate                                            | 105-56-6   | 22.5                          | 11.0                    | m               |
| Ethylene bromide                                              | 593-60-2   | 19.8                          | 9.7                     | p               |
| Ethylene carbonate                                            | 96-49-1    | 30.1                          | 14.7                    | m               |
| Ethylene chlorohydrin (2-chloroethanol)                       | 107-07-3   | 25.0                          | 12.2                    | s               |
| Ethylene cyanohydrin (3-hydroxypropionitrile)                 | 109-78-4   | 31.1                          | 15.2                    | s               |
| Ethylenediamine                                               | 107-15-3   | 25.2                          | 12.3                    | s               |
| Ethylene dichloride (1,2-dichloroethane)                      | 107-06-2   | 20.1                          | 9.8                     | p               |
| Ethylene glycol                                               | 107-21-1   | 29.9                          | 14.6                    | s               |
| Ethylene glycol diacetate                                     | 111-55-7   | 20.5                          | 10.0                    | m               |
| Ethylene glycol diethyl ether                                 | 629-14-1   | 17.0                          | 8.3                     | m               |
| Ethylene glycol dimethyl ether                                | 110-71-4   | 17.6                          | 8.6                     | m               |
| Ethylene glycol methyl ether acetate                          | 110-49-6   | 18.8                          | 9.2                     | m               |
| Ethylene glycol monobenzyl ether                              | 622-08-2   | 22.3                          | 10.9                    | m               |
| Ethylene glycol monobutyl ether                               | 111-76-2   | 19.4                          | 9.5                     | m               |
| Ethylene glycol monoethyl ether (2-ethoxyethanol; Cellusolve) | 110-80-5   | 21.5                          | 10.5                    | m               |
| Ethylene glycol monomethyl ether (2-methoxyethanol)           | 109-86-4   | 23.3                          | 11.4                    | m               |
| Ethylene glycol monophenyl ether                              | 122-99-6   | 23.5                          | 11.5                    | m               |
| Ethylene oxide                                                | 75-21-8    | 22.7                          | 11.1                    | m               |
| Ethylene formamide ( <i>N</i> )                               |            | 28.4                          | 13.9                    | s               |
| Ethyl formate                                                 | 109-94-4   | 19.2                          | 9.4                     | m               |
| Ethyl-2-hexanediol-1,3 (octylene glycol)                      | 94-96-2    | 19.2                          | 9.4                     | s               |
| Ethylhexanol                                                  | 104-76-7   | 19.4                          | 9.5                     | s               |
| Ethyl hexyl acrylate                                          | 103-11-7   | 16.0                          | 7.8                     | m               |
| Ethylidene chloride                                           | 75-34-3    | 18.2                          | 8.9                     | p               |
| Ethyl iodide (iodoethane)                                     | 75-03-6    | 19.2                          | 9.4                     | m               |
| Ethyl isobutyl ether                                          | 627-02-1   | 15.3                          | 7.5                     | m               |
| Ethyl isobutyrate                                             | 97-62-1    | 16.2                          | 7.9                     | m               |
| Ethyl lactate                                                 | 687-47-8   | 20.5                          | 10.0                    | m               |
| Ethyl mercaptan (ethane thiol)                                | 75-08-1    | 18.8                          | 9.2                     | p               |
| Ethyl methacrylate                                            | 97-63-2    | 17.0                          | 8.3                     | m               |
| Ethyl morpholine ( <i>N</i> )                                 | 100-74-3   | 18.2                          | 8.9                     | s               |
| Ethyl orthoformate (triethyl orthoformate)                    | 122-51-0   | 17.0                          | 8.3                     | m               |
| Ethyl propionate                                              | 105-37-3   | 17.2                          | 8.4                     | m               |
| Fluorocarbons, aliphatic                                      |            | 11.3-12.7                     | 5.5-6.2                 | p               |
| Formamide                                                     | 75-12-7    | 15.3-16.8                     | 7.5-8.2                 | p               |
| Formic acid                                                   | 64-18-6    | 39.3                          | 19.2                    | s               |
|                                                               |            | 24.8                          | 12.1                    | s               |

TABLE 7. *cont'd*

| Solvent                                 | Solubility parameter $\delta$ |                    |                         | H-Bonding Group |
|-----------------------------------------|-------------------------------|--------------------|-------------------------|-----------------|
|                                         | CAS number                    | MPa <sup>1/2</sup> | (cal/cm) <sup>1/2</sup> |                 |
| Formylmorpholine ( <i>N</i> )           | 4394-85-8                     | 26.6               | 13.0                    | m               |
| Formylpiperidine ( <i>N</i> )           | 2591-86-8                     | 23.5               | 11.5                    | m               |
| Furan                                   | 110-00-9                      | 19.2               | 9.4                     | m               |
| Furfural (2-furaldehyde)                | 98-01-1                       | 22.9               | 11.2                    | m               |
| Furfuryl alcohol                        | 98-00-0                       | 25.6               | 12.5                    | m               |
| Glycerol                                | 56-81-5                       | 33.8               | 16.5                    | s               |
| Heptane (normal)                        | 142-82-5                      | 15.1               | 7.4                     | s               |
| Heptyl alcohol (normal)                 | 111-70-6                      | 21.7               | 10.6                    | s               |
| Hexamethylphosphoramide                 | 680-31-9                      | 21.5               | 10.5                    | s               |
| Hexane (normal)                         | 110-54-3                      | 14.9               | 7.3                     | s               |
| Hexanediol-2,5                          | 2935-44-6                     | 21.2               | 10.3                    | p               |
| Hexene-1                                | 592-41-6                      | 15.1               | 7.4                     | p               |
| Hexyl alcohol (normal)                  | 111-27-3                      | 21.9               | 10.7                    | p               |
| Hydrazine                               | 302-10-2                      | 37.3               | 18.1                    | s               |
| Hydrogen                                | 1333-74-0                     | 6.9                | 3.0                     | s               |
| Hydrogenated terphenyl (Monsanto HB-40) |                               | 18.4               | 9.0                     | p               |
| Hydrogen cyanide                        | 74-90-8                       | 24.8               | 12.1                    | s               |
| Iodobenzene                             | 591-50-4                      | 20.7               | 10.1                    | p               |
| Isophorone                              | 78-59-1                       | 18.6               | 9.1                     | m               |
| Isoprene                                | 78-79-5                       | 15.1               | 7.4                     | p               |
| Lauryl alcohol                          | 112-53-8                      | 16.6               | 8.1                     | p               |
| Low odor mineral spirits                |                               | 14.1               | 6.9                     | p               |
| Maleic anhydride                        | 108-31-6                      | 27.8               | 13.6                    | s               |
| Malononitrile                           | 109-77-3                      | 30.9               | 15.1                    | p               |
| Mesitylene                              | 108-67-8                      | 18.0               | 8.8                     | p               |
| Mesityl oxide                           | 141-79-7                      | 18.4               | 9.0                     | m               |
| Methacrylic acid                        | 79-41-4                       | 22.9               | 11.2                    | s               |
| Methane                                 | 74-82-8                       | 11.0               | 5.4                     | p               |
| Methanol                                | 67-56-1                       | 29.7               | 14.5                    | s               |
| Methoxy-4-methyl-4-pentanol-2           |                               | 17.4               | 8.5                     | s               |
| Methoxy-4-methyl-4-pentanone-2          | 107-70-0                      | 17.0               | 8.3                     | m               |
| Methylacetamide                         | 79-16-3                       | 29.9               | 14.6                    | s               |
| Methyl acetate                          | 79-20-9                       | 19.6               | 9.6                     | m               |
| Methyl acrylate                         | 96-33-3                       | 18.2               | 8.9                     | m               |
| Methylamine                             | 74-89-5                       | 22.9               | 11.2                    | s               |
| Methyl amyl acetate                     | 108-84-9                      | 16.4               | 8.0                     | m               |
| Methyl amyl ketone                      | 110-43-0                      | 17.4               | 8.5                     | m               |
| Methyl benzoate                         | 95-58-3                       | 21.5               | 10.5                    | m               |
| Methyl bromide                          | 74-83-9                       | 19.6               | 9.6                     | m               |
| Methyl <i>n</i> -butyl ketone           | 591-78-6                      | 17.0               | 8.3                     | m               |
| Methyl <i>n</i> -butyrate               | 623-42-7                      | 18.2               | 8.9                     | m               |
| Methyl caprolactone                     |                               | 18.2               | 8.9                     | m               |
| Methyl chloride                         | 74-87-3                       | 19.8               | 9.7                     | p               |
| Methylcyclohexane                       | 10120-28-2                    | 16.0               | 7.8                     | m               |
| Methylcyclohexanone                     | 589-92-4                      | 19.0               | 9.3                     | m               |
| Methylene chloride                      | 75-09-2                       | 19.8               | 9.7                     | p               |
| Methylene glycolate                     | 61192-32-3                    | 25.4               | 12.4                    | m               |
| Methylene iodide                        | 75-11-6                       | 24.1               | 11.8                    | p               |
| Methyl ethyl ketone                     | 78-93-3                       | 19.0               | 9.3                     | m               |
| Methyl ethyl sulfone                    | 594-43-4                      | 27.4               | 13.4                    | m               |
| Methylformamide ( <i>N</i> )            | 123-39-7                      | 32.9               | 16.1                    | s               |
| Methyl formate                          | 107-31-3                      | 20.9               | 10.2                    | m               |
| Methyl <i>n</i> -hexyl ketone           | 111-13-7                      | 17.0               | 8.3                     | m               |
| Methyl iodide                           | 74-88-4                       | 20.9               | 10.2                    | m               |
| Methyl isoamyl ketone                   | 110-12-3                      | 17.2               | 8.4                     | m               |
| Methyl isobutyl carbinol                | 108-11-2                      | 20.5               | 10.0                    | s               |
| Methyl isobutyl ketone                  | 108-10-1                      | 17.2               | 8.4                     | m               |
| Methyl isobutyrate                      | 547-63-7                      | 17.0               | 8.3                     | m               |
| Methyl isopropyl ketone                 | 563-80-4                      | 17.4               | 8.5                     | m               |
| Methyl isovalerate                      | 624-24-8                      | 16.2               | 7.9                     | m               |
| Methyl methacrylate                     | 80-62-6                       | 18.0               | 8.8                     | m               |
| Methyl nonyl ketone                     | 112-12-9                      | 16.0               | 7.8                     | s               |
| Methyl-2-pentanediol-1,3                | 149-31-5                      | 21.1               | 10.3                    | s               |

TABLE 7. *cont'd*

| Solvent                                              | Solubility parameter $\delta$ |                       |                         | H-bonding group |
|------------------------------------------------------|-------------------------------|-----------------------|-------------------------|-----------------|
|                                                      | CAS number                    | (MPa <sup>1/2</sup> ) | (cal/cm) <sup>1/2</sup> |                 |
| Methyl-2-pentanediol-2,4                             | 107-41-5                      | 19.8                  | 9.7                     | s               |
| Methyl-2-pentanediol monoethyl ether (Pentoxol)      |                               | 17.4                  | 8.5                     | m               |
| Methyl propionate                                    | 554-12-1                      | 18.2                  | 8.9                     | m               |
| Methyl propyl ketone                                 | 107-87-9                      | 17.8                  | 8.7                     | m               |
| Methyl propyl sulfone                                | 1977-37-3                     | 25.6                  | 12.5                    | m               |
| Methyl pyrrolidone-2 (1-methyl-2-pyrrolidinone)      | 872-50-4                      | 23.1                  | 11.3                    | m               |
| Methyl salicylate                                    | 119-36-8                      | 21.7                  | 10.6                    | m               |
| Methyl styrene ( $\alpha$ )                          | 98-83-9                       | 17.4                  | 8.5                     | p               |
| Methyltetramethylene sulfone                         |                               | 26.4                  | 12.9                    | m               |
| Methyl <i>n</i> -valerate                            | 624-24-8                      | 16.2                  | 7.9                     | m               |
| Morpholine                                           | 110-91-8                      | 22.1                  | 10.8                    | s               |
| Naphthalene                                          | 91-20-3                       | 20.3                  | 9.9                     | p               |
| Neopentane                                           | 463-82-1                      | 12.9                  | 6.3                     | p               |
| Neopentyl glycol                                     | 126-30-7                      | 22.5                  | 11.0                    | s               |
| Nitrobenzene                                         | 98-95-3                       | 20.5                  | 10.0                    | p               |
| Nitroethane                                          | 79-24-3                       | 22.7                  | 11.1                    | p               |
| Nitromethane                                         | 75-52-5                       | 26.0                  | 12.7                    | p               |
| Nitro- <i>n</i> -octane                              |                               | 14.3                  | 7.0                     | p               |
| Nitro-1-propane                                      | 108-03-2                      | 21.1                  | 10.3                    | p               |
| Nitro-2-propane                                      | 79-46-9                       | 20.3                  | 9.9                     | p               |
| Nonyl phenol                                         | 25154-52-3                    | 19.2                  | 9.4                     | s               |
| Octane (normal)                                      | 111-65-9                      | 15.6                  | 7.6                     | p               |
| Octyl alcohol (normal)                               | 111-87-5                      | 21.1                  | 10.3                    | s               |
| Pentachloroethane                                    | 76-01-7                       | 19.2                  | 9.4                     | p               |
| Pentane (normal)                                     | 109-66-0                      | 14.3                  | 7.0                     | p               |
| Pentanediol-1,5                                      | 111-29-5                      | 23.5                  | 11.5                    | s               |
| Pentanediol-2,4                                      | 625-69-4                      | 22.1                  | 10.8                    | s               |
| Perchloroethylene                                    | 127-18-4                      | 19.0                  | 9.3                     | p               |
| Perfluoroheptane                                     | 335-57-9                      | 11.9                  | 5.8                     | p               |
| Perfluoromethylcyclohexane                           | 355-02-2                      | 12.3                  | 6.0                     | p               |
| Phenanthrene                                         | 85-01-8                       | 20.1                  | 9.8                     | p               |
| Phenylhydrazine                                      | 100-63-0                      | 25.6                  | 12.5                    | s               |
| Pine oil                                             |                               | 17.6                  | 8.6                     | p               |
| Piperidine                                           | 110-89-4                      | 17.8                  | 8.7                     | p               |
| Piperidone                                           | 675-20-7                      | 27.8                  | 13.6                    | s               |
| Propane                                              | 74-98-6                       | 13.1                  | 6.4                     | p               |
| Propiolactone                                        | 57-57-8                       | 27.2                  | 13.3                    | m               |
| Propionic acid                                       | 79-09-4                       | 20.3                  | 9.9                     | s               |
| Propionic anhydride                                  | 123-62-6                      | 20.5                  | 10.0                    | s               |
| Propionitrile                                        | 107-12-0                      | 22.1                  | 10.8                    | p               |
| Propyl acetate (iso)                                 | 108-21-4                      | 17.2                  | 8.4                     | m               |
| Propyl acetate (normal)                              | 109-60-4                      | 18.0                  | 8.8                     | m               |
| Propyl alcohol (2-propanol)                          | 67-63-0                       | 23.5                  | 11.5                    | s               |
| Propyl alcohol (1-propanol)                          | 71-23-8                       | 24.3                  | 11.9                    | s               |
| Propylbenzene (normal)                               | 103-65-1                      | 17.6                  | 8.6                     | p               |
| Propyl bromide (1-bromopropane)                      | 106-94-5                      | 18.2                  | 8.9                     | m               |
| Propyl butyrate                                      | 105-66-8                      | 17.2                  | 8.4                     | m               |
| Propyl butyrate (iso)                                | 638-11-9                      | 16.2                  | 7.9                     | m               |
| Propyl chloride (2-chloropropane)                    | 75-29-6                       | 16.6                  | 8.1                     | m               |
| Propyl chloride (1-chloropropane)                    | 540-54-5                      | 17.4                  | 8.5                     | m               |
| Propylene-1,2-carbonate                              | 108-32-7                      | 27.2                  | 13.3                    | m               |
| Propylene glycol (1,2-propanediol)                   | 57-55-6                       | 25.8                  | 12.6                    | s               |
| Propylene glycol methyl ether (1,2-dimethoxypropane) | 7778-85-0                     | 20.7                  | 10.1                    | m               |
| Propylene oxide                                      | 75-56-9                       | 18.8                  | 9.2                     | m               |
| Propyl ether (di-, normal)                           | 111-43-3                      | 16.0                  | 7.8                     | m               |
| Propyl ether (iso)                                   | 108-20-3                      | 14.5                  | 7.1                     | m               |
| Propyl formate                                       | 110-74-7                      | 18.8                  | 9.2                     | m               |
| Propyl propionate                                    | 106-36-5                      | 17.4                  | 8.5                     | m               |
| Pyridine                                             | 110-86-1                      | 21.9                  | 10.7                    | s               |
| Pyrene ( $\gamma$ )                                  | 504-31-4                      | 27.4                  | 13.4                    | m               |
| Pyrrolidine ( $\alpha$ ) (iso)                       | 123-75-1                      | 30.1                  | 14.7                    | s               |
| Quinoline                                            | 00-02-2                       | 22.1                  | 10.8                    | s               |
| Santicizer 8                                         |                               | 24.3                  | 11.9                    | m               |



TABLE 7. *cont'd*

| Solvent                                                             | CAS number | Solubility parameter $\delta$ |                         | H-bonding group |
|---------------------------------------------------------------------|------------|-------------------------------|-------------------------|-----------------|
|                                                                     |            | (MPa <sup>1/2</sup> )         | (cal/cm) <sup>1/2</sup> |                 |
| Shell Sol 72                                                        |            | 14.7                          | 7.2                     |                 |
| Shell TS28 solvent                                                  |            | 15.1                          | 7.4                     |                 |
| Silicon tetrachloride                                               |            | 15.1                          | 7.4                     |                 |
| Socal solvent No. 1                                                 |            | 16.6                          | 8.1                     |                 |
| Socal solvent No. 2                                                 |            | 16.2                          | 7.9                     |                 |
| Socal solvent No. 3                                                 |            | 15.8                          | 7.7                     |                 |
| Solvesso 100                                                        |            | 17.6                          | 8.6                     |                 |
| Solvesso 150                                                        |            | 17.4                          | 8.5                     |                 |
| Styrene                                                             | 100-42-5   | 19.0                          | 9.3                     |                 |
| Styrene oxide                                                       | 96-09-3    | 21.5                          | 10.5                    |                 |
| Succinic anhydride                                                  | 108-30-5   | 31.5                          | 15.4                    |                 |
| Terpene B                                                           |            | 17.2                          | 8.4                     |                 |
| Tetrachloroethane-1,1,2,2                                           | 79-34-5    | 19.8                          | 9.7                     |                 |
| Tetrachloroethylene (perchloroethylene)                             | 127-18-4   | 19.0                          | 9.3                     |                 |
| Tetraethylene glycol                                                | 112-60-7   | 20.3                          | 9.9                     |                 |
| Tetrahydrofuran                                                     | 109-99-9   | 18.6                          | 9.1                     |                 |
| Tetrahydronaphthalene (tetralin)                                    | 119-64-2   | 19.4                          | 9.5                     |                 |
| Tetramethylene sulfone (sulfolane, tetrahydrothiophene 1,1-dioxide) | 126-33-0   | 27.4                          | 13.4                    |                 |
| Tetramethyloxamide                                                  |            | 23.3                          | 11.4                    |                 |
| Thiophene                                                           | 110-02-1   | 20.1                          | 9.8                     |                 |
| Toluene                                                             | 108-88-3   | 18.2                          | 8.9                     |                 |
| Tolylene diisocyanate (4-methyl-1,3-phenylene diisocyanate)         | 584-84-9   | 23.7                          | 11.6                    |                 |
| Tributylamine                                                       | 102-82-9   | 15.8                          | 7.7                     |                 |
| Trichloroethane-1,1,2                                               | 79-00-5    | 19.6                          | 9.6                     |                 |
| Trichloroethylene                                                   | 79-01-6    | 18.8                          | 9.2                     |                 |
| Trichlorofluoromethane                                              | 75-69-4    | 15.5                          | 7.6                     |                 |
| Trichlorotrifluoroethane (1,1,2-trichlorotrifluoroethane)           | 76-13-1    | 14.9                          | 7.3                     |                 |
| Tricresyl phosphate (tritolyl phosphate)                            | 1330-78-5  | 17.2                          | 8.4                     |                 |
| Triethylamine                                                       | 121-44-8   | 15.1                          | 7.4                     |                 |
| Triethylene glycol                                                  | 112-27-6   | 21.9                          | 10.7                    |                 |
| Triethylenetetramine                                                | 112-24-3   | 22.7                          | 11.1                    |                 |
| Trimethyl-3,5,5-hexanol (nonyl alcohol)                             | 3452-97-9  | 17.2                          | 8.4                     |                 |
| Triphenyl phosphate                                                 | 115-86-6   | 17.6                          | 8.6                     |                 |
| Triphenyl phosphite                                                 | 101-02-0   | 19.0                          | 9.3                     |                 |
| Tripropylene glycol                                                 | 24800-44-0 | 18.8                          | 9.2                     |                 |
| Tripropylene glycol methyl ether                                    | 20324-33-8 | 17.8                          | 8.7                     |                 |
| Turpentine                                                          | 8006-64-2  | 16.6                          | 8.1                     |                 |
| Valeric acid (normal)                                               | 109-52-4   | 20.1                          | 9.8                     |                 |
| Valeronitrile (normal)                                              | 110-59-8   | 19.6                          | 9.6                     |                 |
| Varnolene (Varsol #2)                                               |            | 15.6                          | 7.6                     |                 |
| Vinyl acetate                                                       | 108-05-4   | 18.4                          | 9.0                     |                 |
| Vinyl chloride                                                      | 75-01-4    | 16.0                          | 7.8                     |                 |
| Vinyl toluene                                                       | 622-97-9   | 18.6                          | 9.1                     |                 |
| V M & P naphtha                                                     |            | 15.6                          | 7.6                     |                 |
| Water                                                               | 7732-18-5  | 47.9                          | 23.4                    |                 |
| Xylene ( <i>p</i> -xylene)                                          | 106-42-3   | 18.0                          | 8.8                     |                 |

TABLE 8. SOLUBILITY PARAMETERS OF SOLVENTS IN INCREASING ORDER OF  $\delta$

| Solvent                            | $\delta$ (MPa <sup>1/2</sup> ) |
|------------------------------------|--------------------------------|
| Hydrogen                           | 6.9                            |
| Dimethyl siloxane                  | 10.0-12.1                      |
| Methane                            | 11.0                           |
| Dichlorodifluoromethane (Freon 12) | 11.3                           |
| Fluorocarbons, aliphatic           | 11.3-12.7                      |
| Perfluoroheptane                   | 11.9                           |
| Ethane                             | 12.3                           |
| Perfluoromethylcyclohexane         | 12.3                           |
| Neopentane                         | 12.9                           |

TABLE 8. *cont'd*

| Solvent                          | $\delta$ (MPa <sup>1/2</sup> ) |
|----------------------------------|--------------------------------|
| Propane                          | 13.1                           |
| Decane (normal)                  | 13.5                           |
| Butylene (iso) (2-methylpropene) | 13.7                           |
| <i>n</i> -Butane                 | 13.9                           |
| Amylene (2-methyl-2-butene)      | 14.1                           |
| Diisopropyl ether                | 14.1                           |
| Low odor mineral spirits         | 14.1                           |
| Nitro- <i>n</i> -octane          | 14.3                           |
| Pentane (normal)                 | 14.3                           |
| 1,3-Butadiene                    | 14.5                           |

TABLE 8. *cont'd*

| Solvent                                                   | $\delta$ (MPa <sup>1/2</sup> ) |
|-----------------------------------------------------------|--------------------------------|
| Propyl ether (iso)                                        | 14.5                           |
| Diisodecyl phthalate                                      | 14.7                           |
| Shell Sol 72                                              | 14.7                           |
| Amyl ether (pentyl ether)                                 | 14.9                           |
| Apco #140 solvent                                         | 14.9                           |
| Ethyl caprylate                                           | 14.9                           |
| Hexane (normal)                                           | 14.9                           |
| Trichlorotrifluoroethane (1,1,2-trichlorotrifluoroethane) | 14.9                           |
| Diethyl ether                                             | 15.1                           |
| Heptane (normal)                                          | 15.1                           |
| Hexene-1                                                  | 15.1                           |
| Isoprene                                                  | 15.1                           |
| Shell TS28 solvent                                        | 15.1                           |
| Silicon tetrachloride                                     | 15.1                           |
| Triethylamine                                             | 15.1                           |
| Apco #18 solvent                                          | 15.3                           |
| Butyl stearate                                            | 15.3                           |
| Ethyl isobutyl ether                                      | 15.3                           |
| Fluorocarbons (aromatic)                                  | 15.3-16.8                      |
| Trichlorofluoromethane                                    | 15.5                           |
| Amyl bromide (1-bromopentane)                             | 15.6                           |
| Octane (normal)                                           | 15.6                           |
| Varnolene (varsol #2)                                     | 15.6                           |
| V M & P naphtha                                           | 15.6                           |
| Diisobutylene                                             | 15.8                           |
| Socal solvent No. 3                                       | 15.8                           |
| Tributylamine                                             | 15.8                           |
| Amyl acetate (iso)                                        | 16.0                           |
| Apco thinner                                              | 16.0                           |
| Butyl (iso) butyrate (normal)                             | 16.0                           |
| Butyl ether                                               | 16.0                           |
| Difluorotetrachloroethane (Freon 112)                     | 16.0                           |
| Diisobutyl ketone                                         | 16.0                           |
| Ethyl hexyl acrylate                                      | 16.0                           |
| Methylcyclohexane                                         | 16.0                           |
| Methyl nonyl ketone                                       | 16.0                           |
| Propyl ether (di-, normal)                                | 16.0                           |
| Vinyl chloride                                            | 16.0                           |
| Dioxane-1,4                                               | 16.2                           |
| Dodecane                                                  | 16.2                           |
| Ethyl isobutyrate                                         | 16.2                           |
| Methyl isovalerate                                        | 16.2                           |
| Methyl <i>n</i> -valerate                                 | 16.2                           |
| Propyl butyrate (iso)                                     | 16.2                           |
| Socal solvent No. 2                                       | 16.2                           |
| Amyl formate (iso)                                        | 16.4                           |
| Dibutoxyethyl phthalate (Kronisol)                        | 16.4                           |
| Diethylamine                                              | 16.4                           |
| Dihexyl ether                                             | 16.4                           |
| Diisopropyl ketone                                        | 16.4                           |
| Methyl amyl acetate                                       | 16.4                           |
| Butyl (normal) butyrate (normal)                          | 16.6                           |
| Butyl chloride (iso) (2-chloro-2-methylpropane)           | 16.6                           |
| Dibutylamine                                              | 16.6                           |
| Lauryl alcohol                                            | 16.6                           |
| Propyl chloride (2-chloropropane)                         | 16.6                           |
| Socal solvent No. 1                                       | 16.6                           |
| Turpentine                                                | 16.6                           |
| <i>sec</i> -Butyl acetate                                 | 16.8                           |
| Butyl formate (iso)                                       | 16.8                           |
| Butyl methacrylate                                        | 16.8                           |
| Cyclohexane                                               | 16.8                           |
| Cymene ( <i>para</i> ) (2-isopropyl toluene)              | 16.8                           |
| Decyl acrylate (iso)                                      | 16.8                           |
| Diacetone alcohol methyl ether (Pentoxone)                | 16.8                           |

TABLE 8. *cont'd*

| Solvent                                         | $\delta$ (MPa <sup>1/2</sup> ) |
|-------------------------------------------------|--------------------------------|
| Dichloropropane-2,2                             | 16.8                           |
| Ethyl amyl ketone (3-octanone)                  | 16.8                           |
| Ethyl benzoate                                  | 16.8                           |
| Ethyl benzoate (secondary)                      | 17.0                           |
| Amyl chloride (1-chloropentane)                 | 17.0                           |
| Butyl acetate (iso)                             | 17.0                           |
| Dichlorofluoromethane (Freon 21)                | 17.0                           |
| Ethylene glycol diethyl ether                   | 17.0                           |
| Ethyl methacrylate                              | 17.0                           |
| Ethyl orthoformate (triethyl orthoformate)      | 17.0                           |
| Methoxy-4-methyl-4-pentanone-2                  | 17.0                           |
| Methyl <i>n</i> -butyl ketone                   | 17.0                           |
| Methyl <i>n</i> -hexyl ketone                   | 17.0                           |
| Methyl isobutyrate                              | 17.0                           |
| Amylformates (normal)                           | 17.2                           |
| Methyl isobutyrate (normal)                     | 17.2                           |
| Amyl iodide (1-iodopentane)                     | 17.2                           |
| Anethole ( <i>para</i> )                        | 17.2                           |
| Benzonitrile                                    | 17.2                           |
| <i>sec</i> -Butyl bromide (2-bromobutane)       | 17.2                           |
| Ethyl propionate                                | 17.2                           |
| Methyl isoamyl ketone                           | 17.2                           |
| Methyl isobutyl ketone                          | 17.2                           |
| Propyl acetate (iso)                            | 17.2                           |
| Propyl butyrate                                 | 17.2                           |
| Terpene B                                       | 17.2                           |
| Tricresyl phosphate (tritolyl phosphate)        | 17.2                           |
| Trimethyl-3,5,5-hexanol (nonyl alcohol)         | 17.2                           |
| Trimethyl-3,5,5-hexanol (normal)                | 17.4                           |
| Bicyclohexyl                                    | 17.4                           |
| <i>n</i> -Butyl acetate                         | 17.4                           |
| Butyl acrylate (iso)                            | 17.4                           |
| Diethylene glycol monobutyl ether acetate       | 17.4                           |
| Diphenyl 2-ethylhexyl phosphate                 | 17.4                           |
| Ethyl <i>n</i> -butyrate                        | 17.4                           |
| Methoxy-4-methyl-4-pentanol-2                   | 17.4                           |
| Methyl amyl ketone                              | 17.4                           |
| Methyl isopropyl ketone                         | 17.4                           |
| Methyl-2-pentanediol monoethyl ether (Pentoxol) | 17.4                           |
| Methyl styrene ( $\alpha$ )                     | 17.4                           |
| Propyl chloride (1-chloropropane)               | 17.4                           |
| Propyl propionate                               | 17.4                           |
| Solvesso 150                                    | 17.4                           |
| Butyl iodide (normal) (1-iodobutane)            | 17.6                           |
| Carbon tetrachloride                            | 17.6                           |
| Diethyl oxalate                                 | 17.6                           |
| Dioxolane-1,3                                   | 17.6                           |
| Dipropylene glycol monomethyl ether             | 17.6                           |
| Ethyl acrylate                                  | 17.6                           |
| Ethylene glycol dimethyl ether                  | 17.6                           |
| Pine oil                                        | 17.6                           |
| Propylbenzene (normal)                          | 17.6                           |
| Solvesso 100                                    | 17.6                           |
| Triphenyl phosphate                             | 17.8                           |
| Amylamine (normal)                              | 17.8                           |
| <i>n</i> -Butylamine                            | 17.8                           |
| <i>n</i> -Butyl bromide (1-bromobutane)         | 17.8                           |
| Cyclopentane                                    | 17.8                           |
| Dibutyl phenyl phosphate                        | 17.8                           |
| Diethylene glycol monolaurate                   | 17.8                           |
| Diocetyl adipate                                | 17.8                           |
| Diocetyl sebacate                               | 17.8                           |
| Methyl propyl ketone                            | 17.8                           |
| Piperidine                                      | 17.8                           |
| Tripropylene glycol methyl ether                | 17.8                           |

TABLE 8. *cont'd*

| Solvent                                                        | $\delta$ (MPa <sup>1/2</sup> ) |
|----------------------------------------------------------------|--------------------------------|
| Aroclor 1248                                                   | 18.0                           |
| Allyl chloride                                                 | 18.0                           |
| <i>n</i> -Butyl acrylate                                       | 18.0                           |
| Butyl propionate                                               | 18.0                           |
| Chlorotoluene ( <i>para</i> )                                  | 18.0                           |
| Decahydronaphthalene ( <i>cis</i> and <i>trans</i> ) (decalin) | 18.0                           |
| Dibutyl sebacate                                               | 18.0                           |
| Diethyl carbonate                                              | 18.0                           |
| Diethyl ketone                                                 | 18.0                           |
| Dimethyl ether                                                 | 18.0                           |
| Ethylbenzene                                                   | 18.0                           |
| Mesitylene                                                     | 18.0                           |
| Methyl methacrylate                                            | 18.0                           |
| Propyl acetate (normal)                                        | 18.0                           |
| Xylene ( <i>p</i> -xylene)                                     | 18.0                           |
| Butyl formate (normal)                                         | 18.2                           |
| Di- <i>n</i> -hexyl phthalate                                  | 18.2                           |
| Ethylidene chloride                                            | 18.2                           |
| Ethyl morpholine (normal)                                      | 18.2                           |
| Methyl acrylate                                                | 18.2                           |
| Methyl <i>n</i> -butyrate                                      | 18.2                           |
| Methyl caprolactone                                            | 18.2                           |
| Methyl propionate                                              | 18.2                           |
| Propyl bromide (1-bromopropane)                                | 18.2                           |
| Toluene                                                        | 18.2                           |
| Butyraldehyde                                                  | 18.4                           |
| Dibutyl fumarate                                               | 18.4                           |
| Dibutyl maleate                                                | 18.4                           |
| Dichloroethylene <i>trans</i> -1,2                             | 18.4                           |
| Dichloropropane-1,2                                            | 18.4                           |
| Hydrogenated terphenyl (Monsanto HB-40)                        | 18.4                           |
| Mesityl oxide                                                  | 18.4                           |
| Vinyl acetate                                                  | 18.4                           |
| Diamyl phthalate                                               | 18.6                           |
| Dichloroethylene, <i>cis</i> -1,2                              | 18.6                           |
| Ethyl acetate                                                  | 18.6                           |
| Isophorone                                                     | 18.6                           |
| Tetrahydrofuran                                                | 18.6                           |
| Vinyl toluene                                                  | 18.6                           |
| Allyl acetate                                                  | 18.8                           |
| Benzene                                                        | 18.8                           |
| Celanese solvent 601                                           | 18.8                           |
| Diacetone alcohol (4-hydroxy-4-methyl-2-pentanone)             | 18.8                           |
| Ethyl chloride                                                 | 18.8                           |
| Ethylene glycol methyl ether acetate                           | 18.8                           |
| Ethyl mercaptan (ethane thiol)                                 | 18.8                           |
| Propylene oxide                                                | 18.8                           |
| Propyl formate                                                 | 18.8                           |
| Trichloroethylene                                              | 18.8                           |
| Tripropylene glycol                                            | 18.8                           |
| Chloroform                                                     | 19.0                           |
| Dibutyl phthalate                                              | 19.0                           |
| Methylcyclohexanone                                            | 19.0                           |
| Methyl ethyl ketone                                            | 19.0                           |
| Perchloroethylene                                              | 19.0                           |
| Styrene                                                        | 19.0                           |
| Tetrachloroethylene (perchloroethylene)                        | 19.0                           |
| Triphenyl phosphite                                            | 19.0                           |
| Benzaldehyde                                                   | 19.2                           |
| Butyl lactate (normal)                                         | 19.2                           |
| Capronitrile (heptyl cyanide)                                  | 19.2                           |
| Dibenzyl ether                                                 | 19.2                           |
| Dimethyl sulfide                                               | 19.2                           |
| Ethyl formate                                                  | 19.2                           |
| Ethyl-2-hexanediol-1,3 (octylene glycol)                       | 19.2                           |

TABLE 8. *cont'd*

| Solvent                                              | $\delta$ (MPa <sup>1/2</sup> ) |
|------------------------------------------------------|--------------------------------|
| Ethyl iodide (iodoethane)                            | 19.2                           |
| Furan                                                | 19.2                           |
| Nonyl phenol                                         | 19.2                           |
| Pentachloroethane                                    | 19.2                           |
| Acetyl chloride                                      | 19.2                           |
| Chlorobenzene                                        | 19.4                           |
| Chlorostyrene ( <i>ortho</i> or <i>para</i> )        | 19.4                           |
| Diethylene glycol monobutyl ether (normal)           | 19.4                           |
| Ethylene glycol monobutyl ether                      | 19.4                           |
| Ethylhexanol                                         | 19.4                           |
| Tetrahydronaphthalene (tetralin)                     | 19.4                           |
| Ethyl bromide (bromoethane)                          | 19.4                           |
| Methyl acetate                                       | 19.6                           |
| Methyl bromide                                       | 19.6                           |
| Trichloroethane-1,1,2                                | 19.6                           |
| Valeronitrile (normal)                               | 19.6                           |
| Chloroethyl acetate ( $\beta$ )                      | 19.8                           |
| Dimethylaniline                                      | 19.8                           |
| Ethylene bromide                                     | 19.8                           |
| Methyl chloride                                      | 19.8                           |
| Methylene chloride                                   | 19.8                           |
| Methyl-2-pentanediol-2,4                             | 19.8                           |
| Tetrachloroethane-1,1,2,2                            | 19.8                           |
| Dodecanol-1                                          | 20-21                          |
| Acrolein                                             | 20.1                           |
| Bromostyrene ( <i>ortho</i> )                        | 20.1                           |
| Butyronitrile (iso)                                  | 20.1                           |
| Dichloroethyl ether                                  | 20.1                           |
| Ethylene dichloride (1,2-dichloroethane)             | 20.1                           |
| Phenanthrene                                         | 20.1                           |
| Thiophene                                            | 20.1                           |
| Valeric acid (normal)                                | 20.1                           |
| Acetone                                              | 20.3                           |
| Anthracene                                           | 20.3                           |
| Bromobenzene                                         | 20.3                           |
| Cyclohexanone                                        | 20.3                           |
| Diethylacetamide ( <i>N,N</i> )                      | 20.3                           |
| Diethyl maleate                                      | 20.3                           |
| Diethyl-2,2-propanediol-1,2 (heptylene glycol)       | 20.3                           |
| Dimethyl carbonate                                   | 20.3                           |
| Naphthalene                                          | 20.3                           |
| Nitro-2-propane                                      | 20.3                           |
| Propionic acid                                       | 20.3                           |
| Tetraethylene glycol                                 | 20.3                           |
| Amyl alcohol                                         | 20.5                           |
| Carbon disulfide                                     | 20.5                           |
| Dichlorobenzene ( <i>ortho</i> )                     | 20.5                           |
| Diethyl phthalate                                    | 20.5                           |
| Dimethyl-2,2-butanediol-1,3                          | 20.5                           |
| Dipentene                                            | 20.5                           |
| Dipropyl phthalate                                   | 20.5                           |
| Ethylamine                                           | 20.5                           |
| Ethylene glycol diacetate                            | 20.5                           |
| Ethyl lactate                                        | 20.5                           |
| Methyl isobutyl carbinol                             | 20.5                           |
| Nitrobenzene                                         | 20.5                           |
| Propionic anhydride                                  | 20.5                           |
| Acetic acid                                          | 20.7                           |
| Caprolactone ( $\epsilon$ )                          | 20.7                           |
| Dibromoethylene-1,2 ( <i>cis</i> and <i>trans</i> )  | 20.7                           |
| Dipropylene glycol                                   | 20.7                           |
| Iodobenzene                                          | 20.7                           |
| Propylene glycol methyl ether (1,2-dimethoxypropane) | 20.7                           |
| Cresol ( <i>meta</i> )                               | 20.9                           |
| Diethylene glycol monobutyl ether                    | 20.9                           |

TABLE 8. *cont'd*

| Solvent                                                       | $\delta$ (MPa <sup>1/2</sup> ) |
|---------------------------------------------------------------|--------------------------------|
| Diphenyl ether                                                | 20.9                           |
| Methyl formate                                                | 20.9                           |
| Methyl iodide                                                 | 20.9                           |
| Acetaldehyde                                                  | 21.1                           |
| Acetic anhydride                                              | 21.1                           |
| Aniline                                                       | 21.1                           |
| Butyric acid (iso) (2-methylpropionic acid)                   | 21.1                           |
| Methyl-2-pentanediol-1,3                                      | 21.1                           |
| Nitro-1-propane                                               | 21.1                           |
| Octyl alcohol (normal)                                        | 21.1                           |
| Hexanediol-2,5                                                | 21.2                           |
| Cyclopentanone                                                | 21.3                           |
| Dibromoethane-1,2                                             | 21.3                           |
| Acrylonitrile                                                 | 21.5                           |
| Butyl alcohol (iso) (2-methyl-1-propanol)                     | 21.5                           |
| Butyric acid (normal)                                         | 21.5                           |
| Butyronitrile (normal)                                        | 21.5                           |
| Ethyl-2-butanol-1                                             | 21.5                           |
| Ethylene glycol monoethyl ether (2-ethoxyethanol; Cellusolve) | 21.5                           |
| Hexamethylphosphoramide                                       | 21.5                           |
| Methyl benzoate                                               | 21.5                           |
| Styrene oxide                                                 | 21.5                           |
| Acetophenone                                                  | 21.7                           |
| 1-Bromonaphthalene                                            | 21.7                           |
| <i>tert</i> -Butyl alcohol (2-methyl-2-propanol)              | 21.7                           |
| Diethylformamide ( <i>N,N</i> )                               | 21.7                           |
| Heptyl alcohol (normal)                                       | 21.7                           |
| Methyl salicylate                                             | 21.7                           |
| Dimethyl phthalate                                            | 21.9                           |
| Hexyl alcohol (normal)                                        | 21.9                           |
| Pyridine                                                      | 21.9                           |
| Triethylene glycol                                            | 21.9                           |
| <i>sec</i> -Butyl alcohol (2-butanol)                         | 22.1                           |
| Dimethylacetamide ( <i>N,N</i> )                              | 22.1                           |
| Morpholine                                                    | 22.1                           |
| Pentanediol-2,4                                               | 22.1                           |
| Propionitrile                                                 | 22.1                           |
| Quinoline                                                     | 22.1                           |
| Quinoline (normal)                                            | 22.3                           |
| Ethylene glycol monobenzyl ether                              | 22.3                           |
| Cyclobutanedione                                              | 22.5                           |
| Dichloroacetic acid                                           | 22.5                           |
| Dimethyl malonate                                             | 22.5                           |
| Dimethyl oxalate                                              | 22.5                           |
| Epichlorohydrin                                               | 22.5                           |
| Ethyl cyanoacetate                                            | 22.5                           |
| Neopentyl glycol                                              | 22.5                           |
| 2,3-Butanediol                                                | 22.7                           |
| Ethylene oxide                                                | 22.7                           |
| Nitroethane                                                   | 22.7                           |
| Triethylenetetramine                                          | 22.7                           |
| Acetylpyrrolidine ( <i>N</i> )                                | 22.7                           |
| Dimethyl-2,2-butanediol-1,2 (isobutylene glycol)              | 22.9                           |
| Furfural (2-furaldehyde)                                      | 22.9                           |
| Methacrylic acid                                              | 22.9                           |
| Methylamine                                                   | 22.9                           |
| Dipropyl sulfone                                              | 23.1                           |
| Methyl pyrrolidone-2 (1-methyl-2-pyrrolidinone)               | 23.1                           |
| Acetylpyrrolidine ( <i>N</i> )                                | 23.1                           |
| <i>n</i> -Butyl alcohol (1-butanol)                           | 23.3                           |
| Cyclohexanol                                                  | 23.3                           |
| Ethylene glycol monomethyl ether (2-methoxyethanol)           | 23.3                           |
| Tetramethyloxamide                                            | 23.3                           |
| Ethylene glycol monophenyl ether                              | 23.5                           |
| Formylpiperidine (normal)                                     | 23.5                           |

TABLE 8. *cont'd*

| Solvent                                                             | $\delta$ (MPa <sup>1/2</sup> ) |
|---------------------------------------------------------------------|--------------------------------|
| Pentanediol-1,5                                                     | 23.5                           |
| Propyl alcohol (2-propanol)                                         | 23.5                           |
| Acetylmorpholine ( <i>N</i> )                                       | 23.7                           |
| 1,3-Butanediol                                                      | 23.7                           |
| Tolylene diisocyanate (4-methyl-1,3-phenylene diisocyanate)         | 23.7                           |
| Allyl alcohol                                                       | 24.1                           |
| Methylene iodide                                                    | 24.1                           |
| Acetonitrile                                                        | 24.3                           |
| Propyl alcohol (1-propanol)                                         | 24.3                           |
| Santicizer 8                                                        | 24.3                           |
| Acrylic acid                                                        | 24.6                           |
| Dimethyltetramethylene sulfone                                      | 24.6                           |
| Benzyl alcohol                                                      | 24.8                           |
| 1,4-Butanediol                                                      | 24.8                           |
| Butylene-2,3 carbonate                                              | 24.8                           |
| Diethylene glycol                                                   | 24.8                           |
| Dimethylformamide ( <i>N,N</i> )                                    | 24.8                           |
| Dioctyl phthalate                                                   | 24.8                           |
| Formic acid                                                         | 24.8                           |
| Hydrogen cyanide                                                    | 24.8                           |
| Ethylene chlorohydrin (2-chloroethanol)                             | 25.0                           |
| Ethylacetamide (normal)                                             | 25.2                           |
| Ethylenediamine                                                     | 25.2                           |
| Diethyl sulfone                                                     | 25.4                           |
| Methylene glycolate                                                 | 25.4                           |
| Dimethyl phosphite                                                  | 25.6                           |
| Furfuryl alcohol                                                    | 25.6                           |
| Methyl propyl sulfone                                               | 25.6                           |
| Phenylhydrazine                                                     | 25.6                           |
| Butyrolactone ( $\gamma$ )                                          | 25.8                           |
| Chloroacetonitrile                                                  | 25.8                           |
| Propylene glycol (1,2-propanediol)                                  | 25.8                           |
| Caprolactam ( $\epsilon$ )                                          | 26.0                           |
| Ethyl alcohol                                                       | 26.0                           |
| Nitromethane                                                        | 26.0                           |
| Methyltetramethylene sulfone                                        | 26.4                           |
| Formylmorpholine ( <i>N</i> )                                       | 26.6                           |
| Dimethylnitroamine ( <i>N,N</i> )                                   | 26.8                           |
| Propiolactone                                                       | 27.2                           |
| Propylene-1,2-carbonate                                             | 27.2                           |
| Methyl ethyl sulfone                                                | 27.4                           |
| Pyrone ( $\gamma$ )                                                 | 27.4                           |
| Tetramethylene sulfone (sulfolane, tetrahydrothiophene 1,1-dioxide) | 27.4                           |
| Maleic anhydride                                                    | 27.8                           |
| Piperidone                                                          | 27.8                           |
| Diacetylpiperazine ( <i>N,N</i> )                                   | 28.0                           |
| Ethylene formamide ( <i>N</i> )                                     | 28.4                           |
| Dimethyl sulfoxide                                                  | 29.7                           |
| Methanol                                                            | 29.7                           |
| Ethylene glycol                                                     | 29.9                           |
| Methylacetamide                                                     | 29.9                           |
| Ethylene carbonate                                                  | 30.1                           |
| Pyrrolidine ( $\alpha$ )                                            | 30.1                           |
| Malononitrile                                                       | 30.9                           |
| Ethylene cyanohydrin (3-hydroxypropionitrile)                       | 31.1                           |
| Diformylpiperazine ( <i>N,N</i> )                                   | 31.5                           |
| Succinic anhydride                                                  | 31.5                           |
| Methylformamide ( <i>N</i> )                                        | 32.9                           |
| Ammonia                                                             | 33.4                           |
| Glycerol                                                            | 33.8                           |
| Hydrazine                                                           | 37.3                           |
| Formamide                                                           | 39.3                           |
| Water                                                               | 47.9                           |

TABLE 9. HANSEN SOLUBILITY PARAMETERS OF LIQUIDS AT 25°C

| Solvent                                    | CAS<br>Number | Molar volume<br>(cm <sup>3</sup> /mol) | Solubility parameters (MPa <sup>1/2</sup> ) |                  |                  |      |
|--------------------------------------------|---------------|----------------------------------------|---------------------------------------------|------------------|------------------|------|
|                                            |               |                                        | δ <sub>d</sub>                              | δ <sub>p</sub>   | δ <sub>h</sub>   | δ    |
| 9.1. PARAFFINIC HYDROCARBONS               |               |                                        |                                             |                  |                  |      |
| <i>n</i> -Butane                           | 106-97-8      | 101.4                                  | 14.1                                        | 0                | 0                | 14.1 |
| <i>n</i> -Pentane                          | 109-66-0      | 116.2                                  | 14.5                                        | 0                | 0                | 14.5 |
| Pentane (iso)                              | 78-78-4       | 117.4                                  | 13.7                                        | 0                | 0                | 13.7 |
| <i>n</i> -Hexane                           | 110-54-3      | 147.4                                  | 14.9                                        | 0                | 0                | 14.9 |
| <i>n</i> -Heptane                          | 142-82-5      | 147.4                                  | 15.3                                        | 0                | 0                | 15.3 |
| <i>n</i> -Octane                           | 111-65-9      | 163.5                                  | 15.6                                        | 0                | 0                | 15.6 |
| 2,2,4-Trimethylpentane                     | 540-84-1      | 166.1                                  | 14.3                                        | 0                | 0                | 14.3 |
| <i>n</i> -Nonane                           | 111-84-2      | 179.7                                  | 15.8                                        | 0                | 0                | 15.8 |
| <i>n</i> -Decane                           | 124-18-5      | 195.9                                  | 15.8                                        | 0                | 0                | 15.8 |
| <i>n</i> -Dodecane                         | 112-40-3      | 228.6                                  | 16                                          | 0                | 0                | 16   |
| <i>n</i> -Hexadecane                       | 544-76-3      | 294.1                                  | 16.4                                        | 0                | 0                | 16.4 |
| <i>n</i> -Eicosane                         | 112-95-8      | 359.8                                  | 16.6                                        | 0                | 0                | 16.6 |
| Cyclohexane                                | 110-82-7      | 108.7                                  | 16.8                                        | 0                | 0.2              | 16.8 |
| Methylcyclohexane                          | 108-87-2      | 128.3                                  | 16                                          | 0                | 1                | 16   |
| <i>cis</i> -Decahydronaphthalene           | 493-01-6      | 156.9                                  | 18.8                                        | 0                | 0                | 18.8 |
| <i>trans</i> -Decahydronaphthalene         | 493-02-7      | 159.9                                  | 18.8                                        | 0                | 0                | 18.8 |
| 9.2. AROMATIC HYDROCARBONS                 |               |                                        |                                             |                  |                  |      |
| Benzene                                    | 71-43-2       | 89.4                                   | 18.4                                        | 0 <sup>a</sup>   | 2                | 18.6 |
| Toluene                                    | 108-88-3      | 106.8                                  | 18                                          | 1.4              | 2                | 18.2 |
| Naphthalene <sup>b</sup>                   | 91-20-3       | 111.5                                  | 19                                          | 2                | 5.9              | 20   |
| Styrene                                    | 1-42-5        | 115.6                                  | 18.6                                        | 1                | 4.1              | 19   |
| <i>o</i> -Xylene                           | 95-47-6       | 121.2                                  | 17.8                                        | 1                | 3.1              | 18   |
| Ethylbenzene                               | 1-41-4        | 123.1                                  | 17.8                                        | 0.6              | 1.4              | 17.8 |
| 1-Methylnaphthalene                        | 90-12-0       | 138.8                                  | 20.6                                        | 0.8              | 4.7              | 21.2 |
| Mesitylene                                 | 108-67-8      | 139.8                                  | 18                                          | 0                | 0.6              | 18   |
| Tetrahydronaphthalene                      | 119-64-2      | 136.0 <sup>a</sup>                     | 19.6 <sup>a</sup>                           | 0                | 2.9              | 20   |
| Biphenyl                                   | 92-52-4       | 154.1                                  | 21.5                                        | 1                | 2                | 21.7 |
| <i>p</i> -Diethylbenzene                   | 105-05-5      | 156.9                                  | 18                                          | 0                | 0.6              | 18   |
| 9.3. HALOHYDROCARBONS                      |               |                                        |                                             |                  |                  |      |
| Methyl chloride                            | 74-87-3       | 55.4                                   | 15.3                                        | 6.1              | 3.9              | 17   |
| Methylene dichloride                       | 75-09-2       | 63.9                                   | 18.2                                        | 6.3              | 6.1              | 20.3 |
| Bromochloromethane                         | 74-97-5       | 65                                     | 17.4                                        | 5.7              | 3.5              | 18.6 |
| Chlorodifluoromethane                      | 75-45-6       | 72.9                                   | 12.3                                        | 6.3              | 5.7              | 14.9 |
| Dichlorofluoromethane                      | 75-43-4       | 75.4                                   | 15.8                                        | 3                | 5.7              | 17   |
| Ethyl bromide                              | 74-96-4       | 76.9                                   | 16.6                                        | 8                | 5.1              | 19   |
| 1,1-Dichloroethylene                       | 75-35-4       | 79                                     | 17                                          | 6.8              | 4.5              | 18.8 |
| Ethylene dichloride                        | 107-06-2      | 79.4                                   | 19.0 <sup>a</sup>                           | 7.4              | 4.1              | 20.9 |
| Methylene diiodide <sup>c</sup>            | 75-11-6       | 80.5                                   | 17.8                                        | 3.9              | 5.5              | 19   |
| Chloroform                                 | 67-66-3       | 80.7                                   | 17.8                                        | 3.1              | 5.7              | 19   |
| 1,1-Dichloroethane                         | 75-34-3       | 84.8                                   | 16.6                                        | 8.2              | 0.4              | 18.4 |
| Ethylene dibromide                         | 106-93-4      | 87                                     | 19.6                                        | 6.8              | 12.1             | 23.9 |
| Bromoform                                  | 75-25-2       | 87.5                                   | 21.5 <sup>a</sup>                           | 4.1              | 6.1 <sup>a</sup> | 22.7 |
| <i>n</i> -Propyl chloride                  | 540-54-5      | 88.1                                   | 16                                          | 7.8              | 2                | 17.8 |
| Trichloroethylene                          | 79-01-6       | 90.2                                   | 18                                          | 3.1              | 5.3              | 19   |
| Dichlorodifluoromethane                    | 75-71-8       | 92.3                                   | 12.3                                        | 2                | 0                | 12.5 |
| Trichlorofluoromethane                     | 75-69-4       | 92.8                                   | 15.3                                        | 2                | 0                | 15.5 |
| Bromotrifluoromethane                      | 75-63-8       | 97                                     | 9.6                                         | 2.5              | 0                | 10   |
| Carbon tetrachloride                       | 56-23-5       | 97.1                                   | 17.8                                        | 0                | 0.6              | 17.8 |
| 1,1,1-Trichloroethane                      | 71-55-6       | 1.4                                    | 17                                          | 4.3              | 2                | 17.6 |
| Tetrachloroethylene                        | 127-18-4      | 101.1                                  | 19                                          | 6.5 <sup>a</sup> | 2.9 <sup>a</sup> | 20.3 |
| Chlorobenzene                              | 108-90-7      | 102.1                                  | 19                                          | 4.3              | 2                | 19.6 |
| <i>n</i> -Butylchloride                    | 109-69-3      | 104.9                                  | 16.4                                        | 5.5              | 2                | 17.4 |
| 1,1,2,2-Tetrachloroethane                  | 79-34-5       | 105.2 <sup>a</sup>                     | 18.8                                        | 5.1              | 9.4              | 21.7 |
| Bromobenzene                               | 222-22-2      | 105.3                                  | 20.5                                        | 5.5              | 4.1              | 21.7 |
| <i>o</i> -Dichlorobenzene                  | 95-50-1       | 112.8                                  | 19.2                                        | 6.3              | 3.3              | 20.5 |
| Benzyl chloride                            | 100-44-7      | 115                                    | 18.8 <sup>a</sup>                           | 7.2              | 2.7              | 20.3 |
| 1,1,2,2-Tetrabromoethane <sup>c</sup>      | 79-27-6       | 116.8                                  | 22.7                                        | 5.1              | 8.2              | 24.8 |
| 1,2-Dichlorotetrafluoroethane <sup>c</sup> | 76-14-2       | 117                                    | 12.7                                        | 1.8              | 0                | 12.9 |
| 1,1,2-Trichlorotrifluoroethane             | 76-13-1       | 119.2                                  | 14.7                                        | 1.6              | 0                | 14.7 |
| Cyclohexyl chloride                        | 542-18-7      | 121.3                                  | 17.4                                        | 5.5              | 2                | 18.4 |

TABLE 9. cont'd

| Solvent                                                | CAS Number | Molar volume (cm <sup>3</sup> /mol) | Solubility parameters (MPa <sup>1/2</sup> ) |                   |                  |      |
|--------------------------------------------------------|------------|-------------------------------------|---------------------------------------------|-------------------|------------------|------|
|                                                        |            |                                     | δ <sub>d</sub>                              | δ <sub>p</sub>    | δ <sub>h</sub>   | δ    |
| 1-Bromonaphthalene                                     | 90-11-9    | 140                                 | 20.3                                        | 3.1               | 4.1              | 20.9 |
| Trichlorobiphenyl <sup>d</sup>                         | 7012-37-5  | 187                                 | 19.2                                        | 5.3               | 4.1              | 20.5 |
| Perfluoromethylcyclohexane                             | 355-02-2   | 196                                 | 12.5                                        | 0                 | 0                | 12.5 |
| Perfluorodimethylcyclohexane                           | 335-27-3   | 217.4                               | 12.5                                        | 0                 | 0                | 12.5 |
| Perfluoro- <i>n</i> -heptane                           | 335-57-9   | 227.3                               | 12.1                                        | 0                 | 0                | 12.5 |
| 9.4. ETHERS                                            |            |                                     |                                             |                   |                  |      |
| Furan                                                  | 110-00-9   | 72.5                                | 17.8                                        | 1.8               | 5.3              | 18.6 |
| Epichlorohydrin                                        | 106-89-8   | 79.9                                | 19                                          | 10.2              | 3.7              | 21.9 |
| Tetrahydrofuran                                        | 109-99-9   | 81.7                                | 16.8                                        | 5.7               | 8                | 19.4 |
| 1,4-Dioxane                                            | 123-91-1   | 85.7                                | 19                                          | 1.8               | 7.4              | 20.5 |
| Methylal (dimethoxymethane)                            | 109-87-5   | 88.8                                | 15.1                                        | 1.8               | 8.6              | 17.6 |
| Diethyl ether                                          | 60-29-7    | 104.8                               | 14.5                                        | 2.9               | 5.1              | 15.8 |
| Bis(2-chloroethyl) ether                               | 107-30-2   | 117.6                               | 18.8                                        | 9                 | 5.7              | 21.7 |
| Anisole                                                | 100-66-3   | 119.1                               | 17.8                                        | 4.1               | 6.8              | 19.4 |
| Bis-(2-methoxyethyl) ether                             | 111-96-6   | 142                                 | 15.8                                        | 6.1               | 9.2              | 19.2 |
| Dibenzyl ether <sup>c</sup>                            | 103-50-4   | 192.7                               | 17.4                                        | 3.7               | 7.4              | 19.2 |
| Di-(chloro-iso-propyl) ether                           | 108-60-1   | 146                                 | 19                                          | 8.2               | 5.1              | 21.3 |
| Bis-( <i>m</i> -phenoxyphenyl) ether                   | 748-30-1   | 373                                 | 19.6                                        | 3.1               | 5.1              | 20.5 |
| 9.5. KETONES                                           |            |                                     |                                             |                   |                  |      |
| Acetone                                                | 67-64-1    | 74                                  | 15.5                                        | 10.4              | 7                | 20.1 |
| Methyl ethyl ketone (2-butanone)                       | 78-93-3    | 90.1                                | 16                                          | 9                 | 5.1              | 19   |
| Cyclohexanone                                          | 108-94-1   | 104                                 | 17.8                                        | 6.3               | 5.1              | 19.6 |
| Diethyl ketone (3-pentanone)                           | 96-22-0    | 106.4                               | 15.8                                        | 7.6               | 4.7              | 18.2 |
| Mesityl oxide (4-methyl-3-pentene-2-one)               | 141-79-7   | 115.6                               | 16.4                                        | 7.2               | 6.1              | 18.8 |
| Acetophenone                                           | 98-86-2    | 117.4                               | 19.6 <sup>a</sup>                           | 8.6               | 3.7              | 21.7 |
| Methyl iso-butyl ketone (2-hexanone)                   | 591-78-6   | 125.8                               | 15.3                                        | 6.1               | 4.1              | 17   |
| Methyl iso-amyl ketone                                 |            | 142.8                               | 16                                          | 5.7               | 4.1              | 17.4 |
| Isophorone                                             | 78-59-1    | 150.5                               | 16.6                                        | 8.2               | 7.4              | 19.8 |
| Di-iso-butyl ketone (2,6-dimethyl-4-heptanone)         | 108-83-8   | 177.1                               | 16                                          | 3.7               | 4.1              | 16.8 |
| 9.6. ALDEHYDES                                         |            |                                     |                                             |                   |                  |      |
| Acetaldehyde                                           | 75-07-0    | 57.1                                | 14.7                                        | 8                 | 11.3             | 20.3 |
| 2-Furfuraldehyde (furfural)                            | 98-01-1    | 83.2                                | 18.6                                        | 14.9              | 5.1              | 24.3 |
| Butyraldehyde                                          | 123-72-8   | 88.5                                | 14.7                                        | 5.3               | 7                | 17.2 |
| Benzaldehyde                                           | 100-52-7   | 101.5                               | 19.4                                        | 7.4               | 5.3              | 21.5 |
| 9.7. ESTERS                                            |            |                                     |                                             |                   |                  |      |
| Ethylene carbonate (1,3-dioxolan-2-one)                | 96-41-9    | 66                                  | 19.4                                        | 21.7              | 5.1              | 29.5 |
| γ-Butyrolactone (4-hydroxybutyric acid γ-lactone)      | 96-48-0    | 76.8                                | 19                                          | 16.6              | 7.4              | 26.2 |
| Methyl acetate                                         | 79-20-9    | 79.7                                | 15.5                                        | 7.2               | 7.6              | 18.8 |
| Ethyl formate                                          | 109-94-4   | 80.2                                | 15.5                                        | 8.4               | 8.4              | 19.6 |
| Propylene carbonate (1,2-propanediol cyclic carbonate) | 108-32-7   | 85                                  | 20.1                                        | 18                | 4.1              | 27.2 |
| Ethyl chloroformate                                    | 541-41-3   | 95.6                                | 15.5                                        | 10                | 6.8              | 19.6 |
| Ethyl acetate                                          | 141-78-6   | 98.5                                | 15.8 <sup>a</sup>                           | 5.3               | 7.2 <sup>a</sup> | 18.2 |
| Trimethyl phosphate                                    | 512-56-1   | 99.9                                | 16.8                                        | 16                | 10.2             | 25.4 |
| Diethyl carbonate                                      | 105-58-8   | 121                                 | 16.6                                        | 3.1               | 6.1              | 18   |
| Diethyl sulfate                                        | 64-67-5    | 131.5                               | 15.8                                        | 14.7              | 7.2              | 22.7 |
| <i>n</i> -Butyl acetate                                | 123-86-4   | 132.5                               | 15.8                                        | 3.7               | 6.3              | 17.4 |
| Iso-butyl acetate                                      | 540-88-5   | 133.5                               | 15.1                                        | 3.7               | 6.3              | 16.8 |
| 2-Ethoxyethyl acetate (Cellusolve acetate)             | 111-15-9   | 136.2                               | 16                                          | 4.7               | 10.6             | 19.6 |
| Iso-amyl acetate                                       | 628-63-7   | 148.8                               | 15.3                                        | 3.1               | 7                | 17.2 |
| Iso-butyl iso-butyrate                                 | 109-21-7   | 163                                 | 15.1                                        | 2.9               | 5.9              | 16.6 |
| Dimethyl phthalate                                     | 131-11-3   | 163                                 | 18.6 <sup>a</sup>                           | 10.8 <sup>a</sup> | 4.9              | 22.1 |
| Ethyl <i>trans</i> -cinnamate                          | 103-36-6   | 166.8                               | 18.4                                        | 8.2               | 4.1              | 20.5 |
| Triethyl phosphate                                     | 78-40-0    | 171                                 | 16.8                                        | 11.5              | 9.2              | 22.3 |
| Diethyl phthalate                                      | 84-66-2    | 198                                 | 17.6                                        | 9.6               | 4.5              | 20.5 |
| Di- <i>n</i> -butyl phthalate                          | 84-74-2    | 266                                 | 17.8 <sup>a</sup>                           | 8.6               | 4.1              | 20.3 |
| <i>n</i> -Butyl benzyl phthalate                       | 85-68-7    | 306                                 | 19                                          | 11.3              | 3.1              | 22.3 |
| Tricresyl phosphate (tritoyl phosphate)                | 1330-78-5  | 613                                 | 19                                          | 12.3              | 4.5              | 23.1 |
| Tri- <i>n</i> -butyl phosphate                         | 126-73-8   | 345                                 | 16.4                                        | 6.3               | 4.3              | 18   |



TABLE 9. *cont'd*

| Solvent                                                                | CAS Number | Molar volume (cm <sup>3</sup> /mol) | Solubility parameters (MPa <sup>1/2</sup> ) |                   |                   |          |
|------------------------------------------------------------------------|------------|-------------------------------------|---------------------------------------------|-------------------|-------------------|----------|
|                                                                        |            |                                     | $\delta_d$                                  | $\delta_p$        | $\delta_h$        | $\delta$ |
| Iso-propyl palmitate <sup>c</sup>                                      | 2239-78-3  | 330                                 | 14.3                                        | 3.9               | 3.7               | 15.3     |
| Di- <i>n</i> -butyl sebacate                                           | 109-43-3   | 339                                 | 14.5                                        | 3.9               | 3.7               | 15.5     |
| Methyl oleate <sup>d</sup>                                             | 112-62-9   | 340                                 | 14.5                                        | 3.9               | 3.7               | 15.5     |
| Diocetyl phthalate (bis(2-ethylhexyl) phthalate)                       | 117-81-7   | 377                                 | 16.6                                        | 7                 | 3.1               | 18.2     |
| Di-butyl stearate <sup>c</sup>                                         |            | 382                                 | 14.5                                        | 3.7               | 3.5               | 15.3     |
| <b>9.8. NITROGEN-CONTAINING COMPOUNDS</b>                              |            |                                     |                                             |                   |                   |          |
| Acetonitrile                                                           | 75-05-8    | 52.6                                | 15.3                                        | 18                | 6.1               | 24.6     |
| Acrylonitrile                                                          | 107-13-1   | 67.1                                | 16.5                                        | 17.4              | 6.8               | 24.8     |
| Propionitrile                                                          | 107-12-0   | 70.9                                | 15.3                                        | 14.3              | 5.5               | 21.7     |
| Butyronitrile                                                          | 109-74-0   | 87                                  | 15.3                                        | 12.5              | 5.1               | 20.5     |
| Benzonitrile                                                           | 100-47-0   | 102.6                               | 17.4                                        | 9                 | 3.3               | 19.8     |
| Nitromethane                                                           | 75-52-5    | 54.3                                | 15.8                                        | 18.8              | 5.1               | 25       |
| Nitroethane                                                            | 79-24-3    | 71.5                                | 16                                          | 15.5              | 4.5               | 22.7     |
| 2-Nitropropane                                                         | 79-46-9    | 86.9                                | 16.2                                        | 12.1              | 4.1               | 20.7     |
| Nitrobenzene                                                           | 98-95-3    | 102.7                               | 20.1                                        | 8.6               | 4.1               | 22.1     |
| Ethanolamine (2-aminoethanol)                                          | 141-43-5   | 60.2                                | 17.2                                        | 15.5              | 21.3              | 31.5     |
| Ethylene diamine                                                       | 107-15-3   | 67.3                                | 16.6                                        | 8.8               | 17                | 25.4     |
| 1,1-Dimethylhydrazine <sup>c</sup>                                     | 57-14-7    | 76                                  | 15.3                                        | 5.9               | 11                | 19.8     |
| 2-Pyrrolidone (2-pyrrolidinone)                                        | 616-45-5   | 76.4                                | 19.4                                        | 17.4              | 11.3              | 28.4     |
| Pyridine                                                               | 110-86-1   | 80.9                                | 19                                          | 8.8               | 5.9               | 21.7     |
| <i>n</i> -Propylamine                                                  | 107-10-8   | 83                                  | 17                                          | 4.9               | 8.6               | 19.6     |
| Morpholine                                                             | 110-91-8   | 87.1                                | 18.8                                        | 4.9               | 9.2               | 21.5     |
| Aniline                                                                | 62-53-3    | 91.5                                | 19.4                                        | 5.1               | 10.2              | 22.5     |
| <i>N</i> -Methyl-2-pyrrolidone (1-methyl-2-pyrrolidinone)              | 872-50-4   | 96.5                                | 18                                          | 12.3              | 7.2               | 22.9     |
| <i>n</i> -Butylamine                                                   | 109-73-9   | 99                                  | 16.2 <sup>a</sup>                           | 4.5 <sup>a</sup>  | 8                 | 18.6     |
| Diethylamine                                                           | 109-87-7   | 103.2                               | 14.9                                        | 2.3               | 6.1               | 16.4     |
| Diethylenetriamine                                                     | 111-40-0   | 108                                 | 16.8                                        | 13.3              | 14.3              | 25.8     |
| Cyclohexylamine                                                        | 108-91-8   | 115.2                               | 17.4                                        | 3.1               | 6.5               | 18.8     |
| Quinoline                                                              | 91-22-5    | 118                                 | 19.4                                        | 7                 | 7.6               | 22.1     |
| Di- <i>n</i> -propylamine                                              | 142-84-7   | 136.9                               | 15.3                                        | 1.4               | 4.1               | 16       |
| Formamide                                                              | 75-12-7    | 39.8                                | 17.2                                        | 26.2              | 19                | 36.6     |
| Dimethylformamide                                                      | 68-12-2    | 77                                  | 17.4                                        | 13.7              | 11.3              | 24.8     |
| <i>N,N</i> -Dimethylacetamide                                          | 127-19-5   | 92.5                                | 16.8                                        | 11.5              | 10.2              | 22.7     |
| 1,1,3,3-Tetramethylurea                                                | 632-22-4   | 120.4                               | 16.8                                        | 8.2               | 11                | 21.7     |
| Hexamethyl phosphoramide <sup>c</sup> (hexamethyl phosphoric triamide) | 680-31-9   | 175.7                               | 18.4                                        | 8.6               | 11.3              | 23.3     |
| <b>9.9. SULFUR-CONTAINING COMPOUNDS</b>                                |            |                                     |                                             |                   |                   |          |
| Carbon disulfide                                                       | 75-15-0    | 60                                  | 20.5                                        | 0                 | 0.6               | 20.5     |
| Dimethyl sulfoxide (methyl sulfoxide)                                  | 67-68-5    | 71.3                                | 18.4                                        | 16.4              | 10.2              | 26.6     |
| Ethanethiol <sup>c</sup> (ethyl mercaptan)                             | 75-08-1    | 74.3                                | 15.8                                        | 6.5               | 7.2               | 18.4     |
| Dimethyl sulfone <sup>b</sup> (methyl sulfone)                         | 67-71-0    | 75                                  | 19                                          | 19.4              | 12.3              | 29.9     |
| Diethyl sulfide (ethyl sulfide)                                        | 352-93-2   | 108.2                               | 17                                          | 3.1               | 2                 | 17.4     |
| <b>9.10. ACID HALIDES AND ANHYDRIDES</b>                               |            |                                     |                                             |                   |                   |          |
| Acetyl chloride                                                        | 75-36-5    | 71                                  | 15.8                                        | 10.6              | 3.9               | 19.4     |
| Succinic anhydride <sup>b</sup>                                        | 108-30-5   | 66.8                                | 18.6                                        | 19.2              | 16.6              | 31.5     |
| Acetic anhydride                                                       | 108-24-7   | 94.5                                | 16.0 <sup>a</sup>                           | 11.7 <sup>a</sup> | 10.2 <sup>a</sup> | 22.3     |
| <b>9.11. ALCOHOLS</b>                                                  |            |                                     |                                             |                   |                   |          |
| Methanol                                                               | 67-56-1    | 40.7                                | 15.1                                        | 12.3              | 22.3              | 29.7     |
| Ethanol                                                                | 64-17-5    | 58.5                                | 15.8                                        | 8.8               | 19.4              | 26.6     |
| Ethylene cyanohydrin (hydracrylonitrile; 3-hydroxypropionitrile)       | 109-78-4   | 68.3                                | 17.2                                        | 18.8              | 17.6              | 30.9     |
| Allyl alcohol (2-propen-1-ol)                                          | 107-18-6   | 68.4                                | 16.2                                        | 10.8              | 16.8              | 25.8     |
| 1-Propanol                                                             | 71-23-8    | 75.2                                | 16                                          | 6.8               | 17.4              | 24.6     |
| 2-Propanol                                                             | 67-63-0    | 76.8                                | 15.8                                        | 6.1               | 16.4              | 23.5     |
| 3-Chloropropanol (trimethylene chlorohydrin)                           | 627-30-5   | 84.2                                | 17.6                                        | 5.7               | 14.7              | 23.7     |
| Furfuryl alcohol                                                       | 98-00-0    | 86.5                                | 17.4                                        | 7.6               | 15.1              | 24.3     |
| 1-Butanol (butyl alcohol)                                              | 71-36-3    | 91.5                                | 16                                          | 5.7               | 15.8              | 23.1     |
| 2-Butanol                                                              | 4221-99-2  | 92                                  | 15.8                                        | 5.7               | 14.5              | 22.1     |

TABLE 9. *cont'd*

| Solvent                                                                        | CAS Number | Molar volume (cm <sup>3</sup> /mol) | Solubility parameters (MPa <sup>1/2</sup> ) |                   |                   |          |
|--------------------------------------------------------------------------------|------------|-------------------------------------|---------------------------------------------|-------------------|-------------------|----------|
|                                                                                |            |                                     | $\delta_d$                                  | $\delta_p$        | $\delta_h$        | $\delta$ |
| 2-Methyl-1-propanol (isobutyl alcohol)                                         | 78-83-1    | 92.8                                | 15.1                                        | 5.7               | 16                | 22.7     |
| Benzyl alcohol                                                                 | 100-51-6   | 103.6                               | 18.4                                        | 6.3               | 13.7              | 23.7     |
| Cyclohexanol                                                                   | 108-93-0   | 106                                 | 17.4                                        | 4.1               | 13.5              | 22.5     |
| 1-Pentanol                                                                     | 71-41-0    | 109                                 | 16                                          | 4.5               | 13.9              | 21.7     |
| 2-Ethyl-1-butanol                                                              | 97-95-0    | 123.2                               | 15.8                                        | 4.3               | 13.5              | 21.3     |
| Diacetone alcohol (4-hydroxy-4-methyl-2-pentanone)                             | 123-42-2   | 124.2                               | 15.8                                        | 8.2               | 10.8              | 20.9     |
| 1,3-Dimethyl-1-butanol                                                         | 105-30-6   | 127.2                               | 15.3                                        | 3.3               | 12.3              | 19.8     |
| Ethyl lactate                                                                  | 687-47-8   | 115                                 | 16                                          | 7.6               | 12.5              | 21.7     |
| <i>n</i> -Butyl lactate                                                        | 138-22-7   | 149                                 | 15.8                                        | 6.5               | 10.2              | 19.8     |
| Ethylene glycol monomethyl ether (2-methoxyethanol)                            | 109-86-4   | 79.1                                | 16.2                                        | 9.2               | 16.4              | 24.8     |
| Ethylene glycol monoethyl ether (2-ethoxyethanol) Cellusolve                   | 111-15-9   | 97.8                                | 16.2                                        | 9.2               | 14.3              | 23.5     |
| Diethylene glycol monomethyl ether (2-(2-methoxyethoxy)ethanol)                | 111-77-3   | 118                                 | 16.2                                        | 9.2               | 12.3              | 22.3     |
| Diethylene glycol monoethyl ether (2-(2-ethoxyethoxy)ethanol)                  | 111-90-0   | 130.9                               | 16.2                                        | 9.2               | 12.3              | 21.9     |
| Ethylene glycol mono- <i>n</i> -butyl ether (2-butoxyethanol) Butyl Cellusolve | 111-76-2   | 131.6                               | 16                                          | 5.1               | 12.3              | 22.3     |
| 2-Ethyl-1-hexanol                                                              | 104-76-7   | 157                                 | 16                                          | 3.3               | 11.9              | 20.1     |
| 1-Octanol (capryl alcohol)                                                     | 111-87-5   | 157.7                               | 17                                          | 3.3               | 11.9              | 20.9     |
| 2-Octanol                                                                      | 123-96-6   | 159.1                               | 16.2                                        | 4.9               | 11                | 20.3     |
| Diethylene glycol mono- <i>n</i> -butyl ether (2-(2-butoxyethoxy)ethanol)      | 112-34-5   | 170.6                               | 16                                          | 7                 | 10.6              | 20.5     |
| 1-Decanol                                                                      | 112-30-1   | 191.8                               | 17.6                                        | 2.7               | 10                | 20.5     |
| Tridecyl alcohol <sup>d</sup>                                                  | 112-70-9   | 242                                 | 14.3                                        | 3.1               | 9                 | 17.2     |
| Nonyl phenoxy ethanol <sup>d</sup>                                             | 27986-36-3 | 275                                 | 16.8                                        | 10.2              | 8.4               | 21.3     |
| Oleyl alcohol <sup>d</sup>                                                     | 143-28-2   | 316                                 | 14.3                                        | 2.7               | 8                 | 16.6     |
| Triethylene glycol mono-oleyl ether                                            |            | 418.5                               | 13.3                                        | 3.1               | 8.4               | 16       |
| <b>9.12. ACIDS</b>                                                             |            |                                     |                                             |                   |                   |          |
| Formic acid                                                                    | 64-18-6    | 37.8                                | 14.3                                        | 11.9              | 16.6              | 25       |
| Acetic acid                                                                    | 64-19-7    | 57.1                                | 14.5                                        | 8                 | 13.5              | 21.3     |
| Benzoic acid <sup>b</sup>                                                      | 65-85-0    | 100                                 | 18.2                                        | 7                 | 9.8               | 21.9     |
| <i>n</i> -Butyric acid <sup>c</sup>                                            | 107-92-6   | 110                                 | 14.9                                        | 4.1               | 10.6              | 18.8     |
| <i>n</i> -Octanoic acid <sup>c</sup>                                           | 124-07-2   | 159                                 | 15.1                                        | 3.3               | 8.2               | 17.6     |
| Oleic acid                                                                     | 112-80-1   | 320                                 | 14.3                                        | 3.1               | 5.5               | 15.8     |
| Stearic acid <sup>b</sup>                                                      | 57-11-4    | 326                                 | 16.4                                        | 3.3               | 5.5               | 17.6     |
| <b>9.13. PHENOLS</b>                                                           |            |                                     |                                             |                   |                   |          |
| Phenol                                                                         | 108-95-2   | 87.5                                | 18                                          | 5.9               | 14.9              | 24.1     |
| 1,3-Benzenediol <sup>b</sup> (resorcinol)                                      | 108-46-3   | 87.5                                | 18                                          | 8.4               | 21.1              | 28.8     |
| <i>m</i> -Cresol                                                               | 108-39-4   | 104.7                               | 18                                          | 5.1               | 12.9              | 22.7     |
| <i>o</i> -Methoxyphenol (guaiacol)                                             | 90-05-1    | 109.5                               | 18                                          | 8.2               | 13.3              | 23.7     |
| Methyl salicylate                                                              | 119-36-8   | 129                                 | 16                                          | 8                 | 12.3              | 21.7     |
| Nonyl phenol <sup>d</sup>                                                      | 25154-52-3 | 231                                 | 16.6                                        | 4.1               | 9.2               | 19.4     |
| <b>9.14. WATER</b>                                                             |            |                                     |                                             |                   |                   |          |
| Water <sup>c</sup>                                                             | 7732-18-5  | 18                                  | 15.5 <sup>a</sup>                           | 16.0 <sup>a</sup> | 42.4 <sup>a</sup> | 47.9     |
| <b>9.15. POLYHYDRIC ALCOHOLS</b>                                               |            |                                     |                                             |                   |                   |          |
| Ethylene glycol                                                                | 107-21-1   | 55.8                                | 17                                          | 11                | 26                | 32.9     |
| Glycerol                                                                       | 56-81-5    | 73.8                                | 17.4                                        | 12.1              | 29.3              | 36.2     |
| Propylene glycol (1,2-propanediol)                                             | 57-55-6    | 73.6                                | 16.8                                        | 9.4               | 23.3              | 30.3     |
| 1,3-Butanediol                                                                 | 107-88-0   | 89.9                                | 16.6                                        | 10                | 21.5              | 28.8     |
| Diethylene glycol                                                              | 111-46-6   | 95.3                                | 16.2                                        | 14.7              | 20.5              | 29.9     |
| Triethylene glycol                                                             | 112-27-6   | 114                                 | 16                                          | 12.5              | 18.6              | 27.4     |
| Hexylene glycol (2-methyl-2,4-pentanediol)                                     | 107-41-5   | 123                                 | 15.8                                        | 8.4               | 17.8              | 25.2     |
| Dipropylene glycol <sup>d</sup>                                                | 110-98-5   | 131.3                               | 16                                          | 20.3              | 18.4              | 31.7     |

<sup>a</sup> Altered from previously published value.<sup>b</sup> Solid, treated as supercooled liquid.<sup>c</sup> Values uncertain.<sup>d</sup> Impure commercial product of this nominal formula.

TABLE 10. SOLUBILITY PARAMETERS OF POLYMERS

| Polymer                                                                       | Molar volume<br>(cm <sup>3</sup> /gmol) | Solubility parameters (MPa) <sup>1/2</sup> |                |                |                                                                             | Method                                                 | T(°C) | Ref. |
|-------------------------------------------------------------------------------|-----------------------------------------|--------------------------------------------|----------------|----------------|-----------------------------------------------------------------------------|--------------------------------------------------------|-------|------|
|                                                                               |                                         | δ <sub>d</sub>                             | δ <sub>p</sub> | δ <sub>h</sub> | δ                                                                           |                                                        |       |      |
| 10.1. MAIN CHAIN CARBON POLYMERS                                              |                                         |                                            |                |                |                                                                             |                                                        |       |      |
| 10.1.1. POLY(DIENES)                                                          |                                         |                                            |                |                |                                                                             |                                                        |       |      |
| Poly(butadiene)                                                               |                                         |                                            |                |                | 14.65<br>17.19<br>17.09<br>17.15<br>17.2–17.6<br>16.6<br>17.6<br>16.2 ± 0.2 | Calc.<br><br><br>Calc.<br>Obs.<br><br><br>IPGC         | 75    |      |
| Emulsion Sodium                                                               |                                         |                                            |                |                | 17.19<br>17.6<br>16.6<br>17.09                                              | <br><br>Calc.<br><br>                                  |       |      |
| Hydrogenated                                                                  |                                         |                                            |                |                | 16.6<br>16.47<br>16.6<br>17.02<br>16.1                                      | Swelling<br><br><br>Av.<br><br><sup>129</sup> Xe shift |       |      |
| Poly(1,2-butadiene)                                                           | 58.85                                   | 16.98                                      | — <sup>a</sup> | 1.02           | 17.06                                                                       | Calc. <sup>HK<sup>b</sup></sup>                        |       |      |
| Poly(3-methyl 1,2-butadiene)                                                  | 73.88                                   |                                            |                |                | 17.39                                                                       | Calc. <sup>HK</sup>                                    |       |      |
| Poly(1,3-butadiene)                                                           | 58.85                                   |                                            |                |                | 17.06                                                                       | Calc. <sup>HK</sup>                                    |       |      |
| Poly(2,3-dimethyl 1,3 butadiene)                                              | 88.91                                   |                                            |                |                | 17.60                                                                       | Calc. <sup>HK</sup>                                    |       |      |
| Poly( <i>cis</i> -butadiene) elastomer (Bunahyls CB10, Chemische Werke Huels) |                                         | 17.53                                      | 2.25           | 3.42           | 18                                                                          |                                                        |       |      |
| Poly(butadiene- <i>co</i> -acrylonitrile)                                     |                                         |                                            |                |                |                                                                             |                                                        |       |      |
| BUNA N (82/18)                                                                |                                         |                                            |                |                | 17.90–17.72                                                                 |                                                        |       |      |
| (82/20)                                                                       |                                         |                                            |                |                | 18.4                                                                        | Calc.                                                  |       |      |
|                                                                               |                                         |                                            |                |                | 19.4                                                                        | Obs.                                                   |       |      |
| BUNA N (75/25)                                                                |                                         |                                            |                |                | 18.93                                                                       | Calc.                                                  | 25    |      |
|                                                                               |                                         |                                            |                |                | 19.19                                                                       | Obs.                                                   |       |      |
|                                                                               |                                         |                                            |                |                | 19.4                                                                        | Obs.                                                   |       |      |
|                                                                               |                                         |                                            |                |                | 18.2                                                                        |                                                        |       |      |
| (70/30)                                                                       |                                         |                                            |                |                | 19.4                                                                        |                                                        |       |      |
|                                                                               |                                         |                                            |                |                | 20.11–20.26                                                                 |                                                        |       |      |
| (61/39)                                                                       |                                         |                                            |                |                | 19.19                                                                       |                                                        |       |      |
|                                                                               |                                         |                                            |                |                | 21.1                                                                        |                                                        |       |      |
|                                                                               |                                         |                                            |                |                | 21.28–21.38                                                                 |                                                        |       |      |
| Hycar (BFGoodrich)                                                            |                                         | 18.6                                       | 8.8            | 4.2            | 20.5 ± 0.6                                                                  | IPGC                                                   | 75    |      |
| Poly(butadiene- <i>co</i> -styrene)                                           |                                         |                                            |                |                | 21                                                                          |                                                        |       |      |
| BUNA S (94/6)                                                                 |                                         |                                            |                |                | 16.45–16.64                                                                 |                                                        |       |      |
| (90/10)                                                                       |                                         |                                            |                |                | 17.13                                                                       |                                                        |       |      |
| (87.5/12.5)                                                                   |                                         |                                            |                |                | 16.39–16.57                                                                 |                                                        |       |      |
|                                                                               |                                         |                                            |                |                | 16.55                                                                       |                                                        |       |      |
|                                                                               |                                         |                                            |                |                | 17.6                                                                        |                                                        |       |      |
| (85/15)                                                                       |                                         |                                            |                |                | 17.31                                                                       |                                                        |       |      |
|                                                                               |                                         |                                            |                |                | 17.19                                                                       |                                                        |       |      |
|                                                                               |                                         |                                            |                |                | 17.35                                                                       | Calc.                                                  |       |      |
|                                                                               |                                         |                                            |                |                | 17.4                                                                        | Obs.                                                   |       |      |
|                                                                               |                                         |                                            |                |                | 17.39                                                                       |                                                        |       |      |
|                                                                               |                                         |                                            |                |                | 17.41                                                                       | Calc.                                                  |       |      |
|                                                                               |                                         |                                            |                |                | 17.39                                                                       | Obs.                                                   |       |      |
|                                                                               |                                         |                                            |                |                | 17.5                                                                        |                                                        |       |      |
| (75/25)                                                                       |                                         |                                            |                |                | 17.29                                                                       |                                                        |       |      |
|                                                                               |                                         |                                            |                |                | 17.47                                                                       | Calc.                                                  |       |      |
|                                                                               |                                         |                                            |                |                | 16.55                                                                       | Obs.                                                   |       |      |
|                                                                               |                                         |                                            |                |                | 16.49                                                                       | Obs.                                                   |       |      |
|                                                                               |                                         |                                            |                |                | 16.6                                                                        |                                                        |       |      |
|                                                                               |                                         |                                            |                |                | 17.5                                                                        |                                                        |       |      |
|                                                                               |                                         |                                            |                |                | 17.56                                                                       | Calc.                                                  |       |      |
|                                                                               |                                         |                                            |                |                | 17.5                                                                        | Obs.                                                   |       |      |
|                                                                               |                                         |                                            |                |                | 17.6                                                                        |                                                        |       |      |

TABLE 10. cont'd

| Polymer                                             | Molar volume<br>(cm <sup>3</sup> /gmol) | Solubility parameters (MPa) <sup>1/2</sup> |                |                |            | Method                  | T(°C) | Refs. |
|-----------------------------------------------------|-----------------------------------------|--------------------------------------------|----------------|----------------|------------|-------------------------|-------|-------|
|                                                     |                                         | δ <sub>d</sub>                             | δ <sub>p</sub> | δ <sub>h</sub> | δ          |                         |       |       |
| Poly(3-methyl 1-butene)                             | 78.12                                   |                                            |                |                | 17.76      | Calc. <sup>HK</sup>     |       | 3     |
| Poly(2-methyl 1-butene)                             | 78.12                                   |                                            |                |                | 17.92      | Calc. <sup>HK</sup>     |       | 3     |
| Poly(2-methyl 2-butene)                             | 78.12                                   |                                            |                |                | 17.68      | Calc. <sup>HK</sup>     |       | 3     |
| Polyethylene                                        |                                         |                                            |                |                | 15.76      |                         |       | 110   |
|                                                     |                                         |                                            |                |                | 16.6       | Calc.                   |       | 112   |
|                                                     |                                         |                                            |                |                | 16         |                         |       | 58    |
|                                                     |                                         |                                            |                |                | 16.2       |                         |       | 97    |
|                                                     |                                         |                                            |                |                | 17.09      |                         |       | 8     |
|                                                     |                                         |                                            |                |                | 16.4       | Calc.                   |       | 124   |
|                                                     |                                         |                                            |                |                | 16.2       |                         |       | 118   |
|                                                     |                                         |                                            |                |                | 16.2       |                         |       | 72    |
|                                                     |                                         |                                            |                |                | 16.8       | Calc.                   |       | 97    |
|                                                     |                                         |                                            |                |                | 16.2       | Obs.                    |       | 73    |
|                                                     |                                         |                                            |                |                | 18.4       | <sup>129</sup> Xe shift |       | 152   |
|                                                     |                                         |                                            |                |                | 17.99      | Calc.                   |       | 119   |
| Poly(ethylene)                                      | 33.03                                   |                                            |                |                | 16.96      | Calc. <sup>HK</sup>     |       | 3     |
| Poly(1,1-diphenyl ethylene)                         | 166.29                                  |                                            |                |                | 19.93      | Calc. <sup>HK</sup>     |       | 3     |
| Poly(methylene)                                     |                                         |                                            |                |                | 14.3       | Extrapol.               | 20    | 45    |
| Poly(ethylene-co-vinyl acetate)                     |                                         |                                            |                |                | 18.6 ± 0.9 | IPGC                    | 25    | 71    |
| Poly(isobutene)                                     |                                         |                                            |                |                | 17.0 ± 0.4 | IPGC                    | 75    | 70    |
|                                                     |                                         |                                            |                |                | 14.5       | Calc.                   |       | 28    |
|                                                     |                                         |                                            |                |                | 16.06      | Av.                     | 35    | 74    |
|                                                     |                                         |                                            |                |                | 16         | Swelling                |       | 74    |
|                                                     |                                         |                                            |                |                | 16.47      | Swelling                |       | 74    |
|                                                     |                                         |                                            |                |                | 16.25      |                         |       | 19,10 |
|                                                     |                                         |                                            |                |                | 16.06      |                         | 25    | 110   |
|                                                     |                                         |                                            |                |                | 15.76      | Calc.                   |       | 112   |
|                                                     |                                         |                                            |                |                | 16.47      | Obs.                    |       | 112   |
|                                                     |                                         |                                            |                |                | 16.4       |                         |       | 58    |
|                                                     |                                         |                                            |                |                | 16.47      |                         |       | 104   |
|                                                     |                                         |                                            |                |                | 16.6       |                         | 21-24 |       |
|                                                     |                                         |                                            |                |                | 16         |                         | 19    |       |
|                                                     |                                         |                                            |                |                | 17         | Calc.                   |       | 124   |
|                                                     |                                         |                                            |                |                | 16.47      |                         |       | 72    |
| Poly(isobutylene) (Lutonal IC/123, BASF)            |                                         | 14.53                                      | 2.52           | 4.66           | 16.47      |                         |       | 79    |
|                                                     |                                         |                                            |                |                | 15.47      |                         |       | 56    |
| Poly(isobutene-co-isoprene) butyl rubber            |                                         |                                            |                |                | 15         | <sup>129</sup> Xe shift |       | 152   |
|                                                     |                                         |                                            |                |                | 15.9-16.06 |                         |       | 19    |
|                                                     |                                         |                                            |                |                | 16.47      |                         |       | 104   |
| Poly(propylene)                                     |                                         |                                            |                |                | 15.76      |                         |       | 112   |
|                                                     |                                         |                                            |                |                | 18.8       |                         | 25    | 58    |
| Poly(propylene)                                     | 48.06                                   |                                            |                |                | 19.2       | Calc.                   |       | 124   |
| Poly(propylene), isotactic (Profax 6701, Hercules)  |                                         | 17.19                                      | -              | -              | 17.49      | Calc. <sup>HK</sup>     |       | 3     |
| Poly(propylene), chlorinated (Parlon P10, Hercules) |                                         | 20.26                                      | 6.32           | 5.4            | 17.19      |                         |       | 81    |
| Poly(2-methyl propene)                              | 63.09                                   |                                            |                |                | 21.89      |                         |       | 56    |
|                                                     |                                         |                                            |                |                | 17.72      | Calc. <sup>HK</sup>     |       | 3     |
| 10.1.3. POLY(ACRYLICS) AND POLY(METHACRYLICS)       |                                         |                                            |                |                |            |                         |       |       |
| Poly(acrylic acid), butyl ester                     |                                         |                                            |                |                | 18         |                         | 35    | 75    |
|                                                     |                                         |                                            |                |                | 18.01      | Av.                     |       | 75    |
|                                                     |                                         |                                            |                |                | 18.52      | Swelling                |       | 75    |
|                                                     |                                         |                                            |                |                | 17.4       | Calc.                   |       | 75    |
|                                                     |                                         |                                            |                |                | 18.6       | Swelling                |       | 77    |
|                                                     |                                         |                                            |                |                | 18.52      |                         |       | 77    |
|                                                     |                                         |                                            |                |                | 19.77      | Calc.                   |       | 119   |
| Poly(acrylic acid), ethyl ester                     |                                         |                                            |                |                | 19.13      | Av.                     |       | 75    |
|                                                     |                                         |                                            |                |                | 19.2       | Swelling                |       | 75    |
|                                                     |                                         |                                            |                |                | 19.8       | Calc.                   |       | 75    |
|                                                     |                                         |                                            |                |                | 19.2       | Swelling                |       | 77    |
|                                                     |                                         |                                            |                |                | 19.13      |                         |       | 77    |
|                                                     |                                         |                                            |                |                | 19.19      |                         |       | 45    |
|                                                     |                                         |                                            |                |                | 18.8       | Calc.                   |       | 62    |
|                                                     |                                         |                                            |                |                | 20.4       | Calc.                   |       | 119   |

TABLE 10. cont'd

| Polymer                                        | Molar volume<br>(cm <sup>3</sup> /gmol) | Solubility parameters (MPa) <sup>1/2</sup> |                |                |             | Method                  | T(°C) | Refs. |
|------------------------------------------------|-----------------------------------------|--------------------------------------------|----------------|----------------|-------------|-------------------------|-------|-------|
|                                                |                                         | δ <sub>d</sub>                             | δ <sub>p</sub> | δ <sub>h</sub> | δ           |                         |       |       |
|                                                |                                         |                                            |                |                | 16.8        | Calc.                   |       | 62    |
| Poly(acrylic acid), isobornyl ester            |                                         |                                            |                |                | 20.7        | Av.                     |       | 75    |
| Poly(acrylic acid), methyl ester               |                                         |                                            |                |                | 20.77       | Swelling                |       | 75    |
|                                                |                                         |                                            |                |                | 20.1        | Calc.                   |       | 75    |
|                                                |                                         |                                            |                |                | 20.77       | Swelling                |       | 77    |
|                                                |                                         |                                            |                |                | 21.3        |                         |       | 77    |
|                                                |                                         |                                            |                |                | 20.7        | Swelling                |       | 75    |
|                                                |                                         |                                            |                |                | 18.52       |                         |       | 75    |
| Poly(acrylic acid), propyl ester               |                                         |                                            |                |                | 18.42       | Av.                     |       | 75    |
|                                                |                                         |                                            |                |                | 18.4        | Calc.                   |       | 75    |
|                                                |                                         |                                            |                |                | 20.7        | Calc.                   |       | 112   |
| Poly(α-chloroacrylic acid), methyl ester       |                                         |                                            |                |                | 17.9        | Swelling                |       | 77    |
| Poly(methacrylic acid), butyl ester            |                                         |                                            |                |                | 17.8        |                         |       | 77    |
|                                                |                                         |                                            |                |                | 18.01       | Swelling                |       | 77    |
|                                                |                                         |                                            |                |                | 17.9        |                         |       | 73    |
|                                                |                                         |                                            |                |                | 17          | Calc.                   |       | 31    |
|                                                |                                         |                                            |                |                | 14.7        | IPGC                    | 140   | 31    |
|                                                |                                         |                                            |                |                | 14.7        | IPGC                    | 140   | 31    |
|                                                |                                         |                                            |                |                | 14.7        | IPGC                    | 140   | 31    |
| Poly(methacrylic acid), isobutyl ester         |                                         |                                            |                |                | 18.4        | Swelling                |       | 77    |
| Poly(methacrylic acid), sec-butyl ester        |                                         |                                            |                |                | 20.3        |                         |       | 77    |
| Poly(methacrylic acid), ethoxyethyl ester      |                                         |                                            |                |                | 18.31       | Swelling                |       | 77    |
| Poly(methacrylic acid), ethyl ester            |                                         |                                            |                |                | 18.2        |                         |       | 77    |
|                                                |                                         |                                            |                |                | 18.6        | Calc.                   |       | 73    |
|                                                |                                         |                                            |                |                | 22.69       |                         |       | 56    |
| Poly(ethyl methacrylate) (Lucite 2042, DuPont) |                                         | 18.64                                      | 10.52          | 7.51           | 20.4        | <sup>129</sup> Xe shift |       | 152   |
|                                                |                                         |                                            |                |                | 17.6        | Calc.                   |       | 73    |
| Poly(methacrylic acid), n-hexyl ester          |                                         |                                            |                |                | 16.6        |                         |       | 62    |
| Poly(methacrylic acid), isobornyl ester        |                                         |                                            |                |                | 16.8        | Calc.                   |       | 73    |
| Poly(methacrylic acid), lauryl ester           |                                         |                                            |                |                | 18.58       |                         | 25    | 19    |
| Poly(methacrylic acid), methyl ester           |                                         |                                            |                |                | 18.52-18.66 |                         |       | 19    |
|                                                |                                         |                                            |                |                | 19.4        | Swelling                |       | 77    |
|                                                |                                         |                                            |                |                | 19.34       |                         |       | 77    |
|                                                |                                         |                                            |                |                | 26.27       |                         |       | 110   |
|                                                |                                         |                                            |                |                | 18.93       | Calc.                   |       | 112   |
|                                                |                                         |                                            |                |                | 18.4-19.4   |                         |       | 7     |
|                                                |                                         |                                            |                |                | 18.58       |                         |       | 118   |
|                                                |                                         |                                            |                |                | 19.5        | Calc.                   |       | 119   |
|                                                |                                         |                                            |                |                | 22.69       |                         |       | 56    |
| Poly(methyl methacrylate) (Rohm and Haas)      |                                         | 18.64                                      | 10.52          | 7.51           | 17.2        | Calc.                   |       | 73    |
| Poly(methacrylic acid), octyl ester            |                                         |                                            |                |                | 18          | Calc.                   |       | 73    |
| Poly(methacrylic acid), propyl ester           |                                         |                                            |                |                | 16          | Calc.                   |       | 73    |
| Poly(methacrylic acid), stearyl ester          |                                         |                                            |                |                | 21          |                         |       | 118   |
| Poly(methacrylonitrile)                        |                                         |                                            |                |                | 21.9        | Calc.                   |       | 112   |
| 10.1.4. POLY(VINYL ALCOHOLS)                   |                                         |                                            |                |                |             |                         |       |       |
| Poly(vinyl alcohol)                            |                                         |                                            |                |                | 25.78       |                         |       | 110   |
|                                                |                                         |                                            |                |                | 21.7        |                         |       | 139   |
|                                                |                                         |                                            |                |                | 22.5        |                         |       | 139   |
| Poly(4-vinyl phenol)                           |                                         |                                            |                |                |             |                         |       |       |
| 10.1.5. POLY(VINYL ESTERS)                     |                                         |                                            |                |                |             |                         |       |       |
| Poly(vinyl acetate)                            |                                         |                                            |                |                | 19.62       | Calc.                   | 25    | 28    |
|                                                |                                         |                                            |                |                | 19.13       |                         | 35    | 78    |
|                                                |                                         |                                            |                |                | 20.93       | Calc.                   |       | 119   |
|                                                |                                         |                                            |                |                | 19.2        | Calc.                   |       | 78    |
|                                                |                                         |                                            |                |                | 18          |                         | 25    | 78    |
|                                                |                                         |                                            |                |                | 22.61       |                         |       | 110   |
|                                                |                                         |                                            |                |                | 19.2        | Calc.                   |       | 112   |
|                                                |                                         |                                            |                |                | 19.2        |                         |       | 118   |
|                                                |                                         |                                            |                |                | 25.66       |                         |       | 56    |
| Poly(vinyl acetate) (Mowilith 50, Hoechst)     |                                         | 20.93                                      | 11.27          | 9.66           | 21.94       | Calc.                   |       | 119   |
| Poly(vinyl acetate-co-vinyl alcohol)           |                                         |                                            |                |                | 23.12       |                         |       | 56    |
| Poly(vinyl butyral) (Butvar B76, Shawinigan)   |                                         | 18.6                                       | 4.36           | 13.03          | 18.01       |                         | 35    | 78    |
| Poly(vinyl propionate)                         |                                         |                                            |                |                | 18.52       | Calc.                   |       | 78    |



TABLE 10. cont'd

| Polymer                                              | Molar volume<br>(cm <sup>3</sup> /gmol) | Solubility parameters (MPa) <sup>1/2</sup> |                |                |             | Method              | T(°C) | Refs. |
|------------------------------------------------------|-----------------------------------------|--------------------------------------------|----------------|----------------|-------------|---------------------|-------|-------|
|                                                      |                                         | δ <sub>d</sub>                             | δ <sub>p</sub> | δ <sub>h</sub> | δ           |                     |       |       |
| 10.1.6. POLY(ALLYL ETHERS) AND POLY(VINYL ETHERS)    |                                         |                                            |                |                |             |                     |       |       |
| Poly(allyl methyl ether)                             | 70.79                                   |                                            |                |                | 19.44       | Calc. <sup>HK</sup> |       | 3     |
| Poly(allyl ethyl ether)                              | 85.82                                   |                                            |                |                | 19.29       | Calc. <sup>HK</sup> |       | 3     |
| Poly(allyl propyl ether)                             | 100.85                                  |                                            |                |                | 19.21       | Calc. <sup>HK</sup> |       | 3     |
| Poly(allyl isopropyl ether)                          | 100.85                                  |                                            |                |                | 19.21       | Calc. <sup>HK</sup> |       | 3     |
| Poly(allyl phenyl ether)                             | 122.39                                  |                                            |                |                | 20.19       | Calc. <sup>HK</sup> |       | 3     |
| Poly(allyl 2, tolyl ether)                           | 137.41                                  |                                            |                |                | 20.03       | Calc. <sup>HK</sup> |       | 3     |
| Poly(allyl 3, tolyl ether)                           | 137.41                                  |                                            |                |                | 20.03       | Calc. <sup>HK</sup> |       | 3     |
| Poly(allyl 4, tolyl ether)                           | 137.41                                  |                                            |                |                | 20.03       | Calc. <sup>HK</sup> |       | 3     |
| Poly(diallyl ether)                                  | 96.61                                   |                                            |                |                | 18.84       | Calc. <sup>HK</sup> |       | 3     |
| Poly(vinyl methyl ether)                             | 55.76                                   |                                            |                |                | 19.66       | Calc. <sup>HK</sup> |       | 3     |
| Poly(vinyl ethyl ether)                              | 70.79                                   |                                            |                |                | 19.44       | Calc. <sup>HK</sup> |       | 3     |
| Poly(vinyl propyl ether)                             | 85.82                                   |                                            |                |                | 19.29       | Calc. <sup>HK</sup> |       | 3     |
| Poly(vinyl butyl ether)                              | 100.85                                  |                                            |                |                | 19.21       | Calc. <sup>HK</sup> |       | 3     |
| Poly(vinyl isopropyl ether)                          | 85.82                                   |                                            |                |                | 19.29       | Calc. <sup>HK</sup> |       | 3     |
| Poly(vinyl isobutyl ether)                           | 100.85                                  |                                            |                |                | 19.21       | Calc. <sup>HK</sup> |       | 3     |
| Poly(vinyl isoamyl ether)                            | 115.88                                  |                                            |                |                | 19.13       | Calc. <sup>HK</sup> |       | 3     |
| Poly(vinyl-1-amyl methyl ether)                      | 119.91                                  |                                            |                |                | 20.83       | Calc. <sup>HK</sup> |       | 3     |
| Poly(vinyl-2-ethyl hexyl ether)                      | 160.96                                  |                                            |                |                | 18.99       | Calc. <sup>HK</sup> |       | 3     |
| Poly(vinyl-2-methoxyethyl ether)                     | 93.52                                   |                                            |                |                | 20.44       | Calc. <sup>HK</sup> |       | 3     |
| Poly(vinyl phenyl ether)                             | 107.36                                  |                                            |                |                | 20.19       | Calc. <sup>HK</sup> |       | 3     |
| Poly(vinyl-1-phenyl methyl ether)                    | 122.39                                  |                                            |                |                | 20.19       | Calc. <sup>HK</sup> |       | 3     |
| Poly(vinyl-1-methyl phenyl ether)                    | 122.39                                  |                                            |                |                | 20.19       | Calc. <sup>HK</sup> |       | 3     |
| Poly(vinyl-1-phenyl phenyl ether)                    | 174.01                                  |                                            |                |                | 20.50       | Calc. <sup>HK</sup> |       | 3     |
| Poly(1-methyl vinyl ethyl ether)                     | 85.82                                   |                                            |                |                | 19.29       | Calc. <sup>HK</sup> |       | 3     |
| Poly(1-ethyl vinyl ethyl ether)                      | 100.85                                  |                                            |                |                | 19.21       | Calc. <sup>HK</sup> |       | 3     |
| Poly(1-phenyl vinyl ethyl ether)                     | 137.41                                  |                                            |                |                | 20.03       | Calc. <sup>HK</sup> |       | 3     |
| Poly(divinyl ether)                                  | 66.55                                   |                                            |                |                | 18.93       | Calc. <sup>HK</sup> |       | 3     |
| 10.1.7. POLY(VINYL HALIDES) AND POLY(VINYL NITRILES) |                                         |                                            |                |                |             |                     |       |       |
| Poly(acrylonitrile)                                  |                                         |                                            |                |                | 25.27       | Calc.               |       | 119   |
|                                                      |                                         |                                            |                |                | 25.6        |                     |       | 66    |
|                                                      |                                         |                                            |                |                | 26.09       | Calc.               | 25    | 112   |
|                                                      |                                         |                                            |                |                | 31.5        |                     |       | 118   |
|                                                      |                                         | 18.21                                      | 16.16          | 6.75           | 25.27       |                     |       | 98    |
| Poly(allyl acetonitrile)                             | 81.13                                   |                                            |                |                | 24.18       | Calc. <sup>HK</sup> |       | 3     |
| Poly(1-methyl acrylonitrile)                         | 66.09                                   |                                            |                |                | 25.45       | Calc. <sup>HK</sup> |       | 3     |
| Poly(2-methyl acrylonitrile)                         | 66.09                                   |                                            |                |                | 25.45       | Calc. <sup>HK</sup> |       | 3     |
| Poly(acrylonitrile-co-isopropyl methacrylate)        |                                         |                                            |                |                | 19.84       |                     |       | 141   |
| Poly(tetrafluoroethylene)                            |                                         |                                            |                |                | 12.7        | Calc.               |       | 112   |
|                                                      |                                         |                                            |                |                | 12.7        |                     |       | 118   |
| Poly(vinyl bromide)                                  |                                         |                                            |                |                | 19.42       |                     |       | 34    |
|                                                      |                                         |                                            |                |                | 19.6        |                     |       | 112   |
| Poly(vinyl chloride)                                 |                                         |                                            |                |                | 19.19–19.34 |                     |       | 19    |
|                                                      |                                         |                                            |                |                | 19.28       | Calc.               |       | 28    |
|                                                      |                                         |                                            |                |                | 20.67       |                     |       | 110   |
|                                                      |                                         |                                            |                |                | 19.54       | Calc.               |       | 112   |
|                                                      |                                         |                                            |                |                | 19.8        | Obs.                |       | 72    |
|                                                      |                                         |                                            |                |                | 19.2        |                     |       | 19    |
|                                                      |                                         |                                            |                |                | 19.8        |                     |       | 21–24 |
|                                                      |                                         |                                            |                |                | 22.1        |                     |       | 58    |
|                                                      |                                         |                                            |                |                | 20.1        |                     |       | 124   |
|                                                      |                                         |                                            |                |                | 19.5        |                     |       | 118   |
|                                                      |                                         |                                            |                |                | 19.8        |                     |       | 72    |
|                                                      |                                         |                                            |                |                | 20.32       | Calc.               |       | 119   |
| Poly(vinyl chloride) (Vipla KR, K = 50, Montecatini) | 18.23                                   | 7.53                                       | 8.35           |                | 21.42       |                     |       | 56    |
| Poly(vinyl chloride)                                 | 18.72                                   | 10.03                                      | 3.07           |                | 21.46       |                     |       | 33    |
|                                                      | 18.82                                   | 10.03                                      | 3.07           |                | 21.54       |                     |       | 98    |
| Poly(vinyl chloride), high molecular weight          |                                         |                                            |                |                | 20.13       | Turbidity           |       | 162   |
|                                                      |                                         |                                            |                |                | 20.25       | Swelling            |       | 162   |
|                                                      |                                         |                                            |                |                | 20.3        | Visc.               |       | 162   |
| Poly(vinyl chloride), chlorinated                    |                                         |                                            |                |                | 19          | Visc.               | 25    | 117   |

TABLE 10. cont'd

| Polymer                                                | Molar volume<br>(cm <sup>3</sup> /gmol) | Solubility parameters (MPa) <sup>1/2</sup> |                |                |             | Method              | T(°C) | Refs. |
|--------------------------------------------------------|-----------------------------------------|--------------------------------------------|----------------|----------------|-------------|---------------------|-------|-------|
|                                                        |                                         | δ <sub>d</sub>                             | δ <sub>p</sub> | δ <sub>h</sub> | δ           |                     |       |       |
| Poly(vinyl chloride-co-vinyl acetate) (87/13)          |                                         |                                            |                |                | 21.7        | Calc.               |       | 28    |
|                                                        |                                         |                                            |                |                | 21.3        |                     |       | 21–24 |
|                                                        |                                         |                                            |                |                | 20.42       | Calc.               |       | 119   |
| VYHH                                                   |                                         |                                            |                |                | 20.44       | Calc.               |       | 119   |
| Poly(vinyl chloride-co-vinyl acetate-co-maleic acid)   |                                         |                                            |                |                | 20.77       | Calc.               |       | 119   |
| Poly(vinyl chloride-co-vinyl acetate-co-vinyl alcohol) | 66.09                                   |                                            |                |                | 25.45       | Calc. <sup>HK</sup> |       | 3     |
| Poly(allyl cyanide)                                    | 66.09                                   |                                            |                |                | 25.45       | Calc. <sup>HK</sup> |       | 3     |
| Poly(allyl isocyanide)                                 |                                         |                                            |                |                | 25          |                     |       | 21–24 |
| Poly(vinylidene chloride)                              |                                         |                                            |                |                | 22.67       | Calc.               |       | 128   |
| Poly(vinylidene cyanide-co-vinyl acetate)              |                                         |                                            |                |                | 23.2        | Visc.               |       | 147   |
| Poly(vinylidene fluoride)                              |                                         | 17.2                                       | 12.5           | 9.2            | 23.2        | Obs.                |       | 147   |
|                                                        |                                         | 16.6, 17.9                                 |                |                |             | Calc.               |       | 147   |
|                                                        |                                         | 16.6                                       |                |                |             | Refract. index      |       | 147   |
|                                                        |                                         | 13.7                                       | 10.6           | 8.2            | 19.2        | Contact ang.        |       | 149   |
|                                                        |                                         |                                            |                |                | 24.6, 25.2  | Swelling            |       | 148   |
| 10.1.8. POLY(STYRENES)                                 |                                         |                                            |                |                |             |                     |       |       |
| Poly(styrene)                                          |                                         |                                            |                |                | 17.52       |                     |       | 19    |
|                                                        |                                         |                                            |                |                | 17.45–17.58 |                     |       | 19    |
|                                                        |                                         |                                            |                |                | 20.16       | Calc.               |       | 28    |
|                                                        |                                         |                                            |                |                | 17.86–17.92 |                     |       | 48    |
|                                                        |                                         |                                            |                |                | 17.84–18.56 | Visc.               |       | 116   |
|                                                        |                                         |                                            |                |                | 18.6        |                     |       | 66    |
|                                                        |                                         |                                            |                |                | 18.72       |                     | 35    | 74    |
|                                                        |                                         |                                            |                |                | 18.62       | Av.                 |       | 74    |
|                                                        |                                         |                                            |                |                | 18.62       | Swelling            |       | 74    |
|                                                        |                                         |                                            |                |                | 18.66       | Calc.               |       | 74    |
|                                                        |                                         |                                            |                |                | 19.09       |                     | 25    | 110   |
|                                                        |                                         |                                            |                |                | 18.66       | Calc.               |       | 112   |
|                                                        |                                         |                                            |                |                | 18.6        | Obs.                |       | 112   |
|                                                        |                                         |                                            |                |                | 17.6–19.8   | Obs.                |       | 112   |
|                                                        |                                         |                                            |                |                | 17.4        |                     |       | 18    |
|                                                        |                                         |                                            |                |                | 17.6        |                     |       | 19    |
|                                                        |                                         |                                            |                |                | 18.4        |                     |       | 58    |
|                                                        |                                         |                                            |                |                | 19.28       | Calc.               |       | 119   |
|                                                        |                                         |                                            |                |                | 21.1        | Calc.               |       | 124   |
|                                                        |                                         |                                            |                |                | 17.52       |                     |       | 118   |
|                                                        |                                         |                                            |                |                | 17.84       |                     |       | 19,97 |
|                                                        |                                         |                                            |                |                | 18.6        |                     |       | 104   |
|                                                        |                                         |                                            |                |                | 17.6–17.8   |                     |       | 72    |
|                                                        |                                         |                                            |                |                | 18.6        |                     |       | 79    |
|                                                        |                                         |                                            |                |                | 15.6        | IPGC                | 140   | 31    |
| Poly(styrene) (Polystyrene LG, BASF)                   |                                         | 21.28                                      | 5.75           | 4.3            | 22.47       |                     |       | 56    |
| Poly(o-methyl styrene)                                 | 114.69                                  |                                            |                |                | 19.33       | Calc. <sup>HK</sup> |       | 3     |
| Poly(m-methyl styrene)                                 | 114.69                                  |                                            |                |                | 19.33       | Calc. <sup>HK</sup> |       | 3     |
| Poly(p-methyl styrene)                                 | 114.69                                  |                                            |                |                | 19.33       | Calc. <sup>HK</sup> |       | 3     |
| Poly(1-methyl styrene)                                 | 114.69                                  |                                            |                |                | 19.33       | Calc. <sup>HK</sup> |       | 3     |
| Poly(methoxy styrene)                                  | 122.39                                  |                                            |                |                | 20.19       | Calc. <sup>HK</sup> |       | 3     |
| Poly(cyano styrene)                                    | 124.28                                  |                                            |                |                | 22.36       | Calc. <sup>HK</sup> |       | 3     |
| Poly(nitro styrene)                                    | 113.29                                  |                                            |                |                | 22.71       | Calc. <sup>Sc</sup> |       | 3     |
| Poly(2-nitro styrene)                                  | 113.29                                  |                                            |                |                | 22.20       | Calc. <sup>S</sup>  |       | 3     |
| Poly(styrene-co-divinylbenzene)                        |                                         |                                            |                |                | 18.6        | Obs.                |       | 112   |
|                                                        |                                         |                                            |                |                | 17.39       |                     |       | 18    |
| 5% crosslinking                                        |                                         |                                            |                |                | 14.8        |                     |       | 137   |
| 10% crosslinking                                       |                                         |                                            |                |                | 15.7        |                     |       | 137   |
| 20% crosslinking                                       |                                         |                                            |                |                | 17.8        |                     |       | 137   |
| Poly(styrene-co-n-butyl methacrylate)                  |                                         |                                            |                |                | 15.1        | IPGC                | 140   | 31    |
| Poly(styrene-co-isobutyl methacrylate)                 |                                         |                                            |                |                | 15.1        | IPGC                | 140   | 31    |
| Poly(4-chlorostyrene)                                  | 17.6                                    | 6.1                                        | 4.1            |                | 19.02       |                     |       | 151   |
| Poly(α-methylstyrene-co-acrylonitrile)                 |                                         |                                            |                |                | 16.4        | IPGC                | 140   | 111   |
| Poly(4-acetoxystyrene)                                 | 17.8                                    | 9                                          | 8.4            |                | 21.7        |                     |       | 138   |
| Poly(4-hydroxystyrene)                                 | 17.6                                    | 10                                         | 13.7           |                | 24.55       |                     |       | 138   |

TABLE 10. cont'd

| Polymer                                                                                                                                                                                                                          | Molar volume<br>(cm <sup>3</sup> /gmol) | Solubility parameters (MPa) <sup>1/2</sup> |                |                |       | Method   | T(°C) | Refs. |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------|--------------------------------------------|----------------|----------------|-------|----------|-------|-------|
|                                                                                                                                                                                                                                  |                                         | δ <sub>d</sub>                             | δ <sub>p</sub> | δ <sub>h</sub> | δ     |          |       |       |
| Poly(4-α-acetoxystyrene),<br>-CH <sub>2</sub> -C-(OCOCH <sub>3</sub> )-(C <sub>6</sub> H <sub>5</sub> -OCOR)-,<br>R=CH <sub>3</sub> , C <sub>2</sub> H <sub>5</sub> , <i>n</i> -C <sub>3</sub> H <sub>7</sub> , OCH <sub>3</sub> |                                         | 15.7                                       | 10.2           | 7.4            | 21.9  |          |       | 161   |
| Poly(vinylidene cyanide-co-4-α-acetoxystyrene),<br>-CH <sub>2</sub> -C(CN) <sub>2</sub> -CH <sub>2</sub> -C-(OCOCH <sub>3</sub> )-<br>(C <sub>6</sub> H <sub>5</sub> -OCOR)-, R=CH <sub>3</sub>                                  | 21.5                                    |                                            | 11.3           | 7.2            | 25.3  |          |       | 161   |
| Poly(vinylidene cyanide-co-4-α-acetoxystyrene),<br>R=OCOCH <sub>3</sub>                                                                                                                                                          | 17                                      |                                            | 13.5           | 6.5            | 23.5  |          |       | 161   |
| Poly(vinylidene cyanide-co-4-α-acetoxystyrene),<br>R=OCOCH <sub>3</sub>                                                                                                                                                          | 17                                      |                                            | 12.1           | 8.2            | 22.4  |          |       | 161   |
| Poly(vinylidene cyanide-co-4-α-acetoxystyrene),<br>R=OCOCH <sub>3</sub>                                                                                                                                                          | 17                                      |                                            | 11.9           | 7.2            | 21.9  |          |       | 161   |
| 10.2. MAIN CHAIN C-O POLYMERS                                                                                                                                                                                                    |                                         |                                            |                |                |       |          |       |       |
| 10.2.1. POLY(ESTERS)                                                                                                                                                                                                             |                                         |                                            |                |                |       |          |       |       |
| Poly(vinyl acetate)                                                                                                                                                                                                              | 74.25                                   |                                            |                |                | 18.21 | Calc. HK |       | 3     |
| Poly(allyl acetate)                                                                                                                                                                                                              | 89.28                                   |                                            |                |                | 18.27 | Calc. HK |       | 3     |
| Poly(diethylaminoethyl acrylate)-palladium ion                                                                                                                                                                                   |                                         |                                            |                |                | 20.50 |          |       | 136   |
| Poly(methyl acrylate)                                                                                                                                                                                                            | 74.25                                   |                                            |                |                | 18.21 | Calc. HK |       | 3     |
| Poly(ethyl acrylate)                                                                                                                                                                                                             | 89.28                                   |                                            |                |                | 18.27 | Calc. HK |       | 3     |
| Poly(allyl acrylate)                                                                                                                                                                                                             | 100.07                                  |                                            |                |                | 17.94 | Calc. HK |       | 3     |
| Poly(butyl acrylate)                                                                                                                                                                                                             | 119.34                                  |                                            |                |                | 20.42 | Calc. HK |       | 3     |
| Poly(isobutyl acrylate)                                                                                                                                                                                                          | 119.34                                  |                                            |                |                | 18.37 | Calc. HK |       | 3     |
| Poly(2-ethyl hexyl acrylate)                                                                                                                                                                                                     | 179.46                                  |                                            |                |                | 18.45 | Calc. HK |       | 3     |
| Poly(2-cyanoethyl acrylate) <sup>a</sup>                                                                                                                                                                                         | 89.36                                   |                                            |                |                | 31.77 | Calc. HK |       | 3     |
| Poly(benzyl acrylate)                                                                                                                                                                                                            | 140.88                                  |                                            |                |                | 19.38 | Calc. HK |       | 3     |
| Poly(vinyl butyrate)                                                                                                                                                                                                             | 104.31                                  |                                            |                |                | 18.33 | Calc. HK |       | 3     |
| Poly(dimethyl citraconate)                                                                                                                                                                                                       | 130.5                                   |                                            |                |                | 18.58 | Calc. HK |       | 3     |
| Poly(diethyl citraconate)                                                                                                                                                                                                        | 160.58                                  |                                            |                |                | 18.58 | Calc. HK |       | 3     |
| Poly(vinyl crotonate)                                                                                                                                                                                                            | 100.07                                  |                                            |                |                | 17.94 | Calc. HK |       | 3     |
| Poly(methyl dimethyl fumarate)                                                                                                                                                                                                   | 130.5                                   |                                            |                |                | 18.58 | Calc. HK |       | 3     |
| Poly(methyl diethyl fumarate)                                                                                                                                                                                                    | 160.56                                  |                                            |                |                | 18.58 | Calc. HK |       | 3     |
| Poly(dimethyl fumarate)                                                                                                                                                                                                          | 115.47                                  |                                            |                |                | 18.56 | Calc. HK |       | 3     |
| Poly(diethyl fumarate)                                                                                                                                                                                                           | 145.53                                  |                                            |                |                | 18.58 | Calc. HK |       | 3     |
| Poly(dipropyl fumarate)                                                                                                                                                                                                          | 165.58                                  |                                            |                |                | 19.72 | Calc. HK |       | 3     |
| Poly(di- <i>n</i> -butyl fumarate)                                                                                                                                                                                               | 205.65                                  |                                            |                |                | 18.60 | Calc. HK |       | 3     |
| Poly(di- <i>n</i> -amyl fumarate)                                                                                                                                                                                                | 235.71                                  |                                            |                |                | 18.60 | Calc. HK |       | 3     |
| Poly(di-isopropyl fumarate)                                                                                                                                                                                                      | 165.58                                  |                                            |                |                | 19.72 | Calc. HK |       | 3     |
| Poly(di-isobutyl fumarate)                                                                                                                                                                                                       | 205.65                                  |                                            |                |                | 18.60 | Calc. HK |       | 3     |
| Poly(di-isoamyl fumarate)                                                                                                                                                                                                        | 235.71                                  |                                            |                |                | 18.60 | Calc. HK |       | 3     |
| Poly(dinitrile fumarate)                                                                                                                                                                                                         | 46.32                                   |                                            |                |                | 48.45 | Calc. HK |       | 3     |
| Poly(diphenyl fumarate)                                                                                                                                                                                                          | 217.67                                  |                                            |                |                | 19.91 | Calc. HK |       | 3     |
| Poly(vinyl-2-ethyl hexoate)                                                                                                                                                                                                      | 157.83                                  |                                            |                |                | 19.21 | Calc. HK |       | 3     |
| Poly(dimethyl maleate)                                                                                                                                                                                                           | 115.47                                  |                                            |                |                | 18.56 | Calc. HK |       | 3     |
| Poly(diethyl maleate)                                                                                                                                                                                                            | 145.53                                  |                                            |                |                | 18.58 | Calc. HK |       | 3     |
| Poly(di- <i>n</i> -propyl maleate)                                                                                                                                                                                               | 165.58                                  |                                            |                |                | 19.70 | Calc. HK |       | 3     |
| Poly(di- <i>n</i> -butyl maleate)                                                                                                                                                                                                | 205.65                                  |                                            |                |                | 18.60 | Calc. HK |       | 3     |
| Poly(di- <i>n</i> -amyl maleate)                                                                                                                                                                                                 | 235.71                                  |                                            |                |                | 18.60 | Calc. HK |       | 3     |
| Poly(di-isobutyl maleate)                                                                                                                                                                                                        | 205.65                                  |                                            |                |                | 18.60 | Calc. HK |       | 3     |
| Poly(di-isoamyl maleate)                                                                                                                                                                                                         | 235.71                                  |                                            |                |                | 18.60 | Calc. HK |       | 3     |
| Poly(diphenyl maleate)                                                                                                                                                                                                           | 217.67                                  |                                            |                |                | 19.91 | Calc. HK |       | 3     |
| Poly(3-chloropropyl methacrylate)                                                                                                                                                                                                |                                         |                                            |                |                | 19.60 |          |       | 160   |
| Poly(methyl methacrylate)                                                                                                                                                                                                        | 89.28                                   |                                            |                |                | 18.27 | Calc. HK |       | 3     |
| Poly(ethyl methacrylate)                                                                                                                                                                                                         | 110.9                                   |                                            |                |                | 17.25 | Calc. HK |       | 3     |
| Poly(propyl methacrylate)                                                                                                                                                                                                        | 119.34                                  |                                            |                |                | 18.37 | Calc. HK |       | 3     |
| Poly(butyl methacrylate)                                                                                                                                                                                                         | 134.37                                  |                                            |                |                | 18.41 | Calc. HK |       | 3     |
| Poly(hexyl methacrylate)                                                                                                                                                                                                         | 191.91                                  |                                            |                |                | 15.80 | Calc. HK |       | 3     |
| Poly(allyl methacrylate)                                                                                                                                                                                                         | 115.1                                   |                                            |                |                | 17.51 | Calc. S  |       | 3     |
| Poly(isopropyl methacrylate)                                                                                                                                                                                                     | 119.34                                  |                                            |                |                | 18.39 | Calc. HK |       | 3     |
| Poly(isobutyl methacrylate)                                                                                                                                                                                                      | 134.37                                  |                                            |                |                | 18.39 | Calc. HK |       | 3     |
| Poly(vinyl propionate)                                                                                                                                                                                                           | 89.32                                   |                                            |                |                | 18.27 | Calc. HK |       | 3     |

TABLE 10. cont'd

| Polymer                                                      | Molar volume<br>(cm <sup>3</sup> /gmol) | Solubility parameters (MPa) <sup>1/2</sup> |                |                |       | Method                         | T(°C) | Refs. |
|--------------------------------------------------------------|-----------------------------------------|--------------------------------------------|----------------|----------------|-------|--------------------------------|-------|-------|
|                                                              |                                         | δ <sub>d</sub>                             | δ <sub>p</sub> | δ <sub>h</sub> | δ     |                                |       |       |
| 10.3. MAIN CHAIN C-N POLYMERS                                |                                         |                                            |                |                |       |                                |       |       |
| 10.3.1. POLY(AMIDES)                                         |                                         |                                            |                |                |       |                                |       |       |
| Poly(lactams)                                                |                                         |                                            |                |                | 26.2  | Calc.                          |       | 139   |
| Nylon 3                                                      |                                         |                                            |                |                | 23.9  | Calc.                          |       | 139   |
| Nylon 4                                                      |                                         | 19.44                                      | — <sup>a</sup> | 14.12          | 24.02 |                                |       | 81    |
|                                                              |                                         |                                            |                |                | 22.5  | Calc.                          |       | 139   |
| Nylon 5                                                      |                                         |                                            |                |                | 21.5  | Calc.                          |       | 139   |
| Nylon 6                                                      |                                         |                                            |                |                | 20.7  | Calc.                          |       | 139   |
| Nylon 7                                                      |                                         |                                            |                |                | 20.3  | Calc.                          |       | 139   |
| Nylon 8                                                      |                                         |                                            |                |                | 19.8  | Calc.                          |       | 139   |
| Nylon 9                                                      |                                         |                                            |                |                | 19.4  | Calc.                          |       | 139   |
| Nylon 10                                                     |                                         |                                            |                |                | 19.2  | Calc.                          |       | 139   |
| Nylon 11                                                     |                                         |                                            |                |                | 19    | Calc.                          |       | 139   |
| Nylon 12                                                     |                                         |                                            |                |                | 27.2  | Calc.                          |       | 139   |
| Nylon 2-I                                                    |                                         |                                            |                |                | 26    | Calc.                          |       | 139   |
| Nylon 3-I                                                    |                                         |                                            |                |                | 25    | Calc.                          |       | 139   |
| Nylon 4-I                                                    |                                         |                                            |                |                | 24.1  | Calc.                          |       | 139   |
| Nylon 5-I                                                    |                                         |                                            |                |                | 23.5  | Calc.                          |       | 139   |
| Nylon 6-I                                                    |                                         |                                            |                |                | 26.3  | Calc. <sup>HK</sup>            |       | 150   |
| Nylon 6I, poly(hexamethylene isophthalamide)                 |                                         |                                            |                |                | 23.2  | Calc. <sup>H<sup>d</sup></sup> |       | 150   |
|                                                              |                                         |                                            |                |                | 22.9  | Calc.                          |       | 139   |
| Nylon 7-I                                                    |                                         |                                            |                |                | 22.5  | Calc.                          |       | 139   |
| Nylon 8-I                                                    |                                         |                                            |                |                | 22.1  | Calc.                          |       | 139   |
| Nylon 9-I                                                    |                                         |                                            |                |                | 21.7  | Calc.                          |       | 139   |
| Nylon 10-I                                                   |                                         |                                            |                |                | 21.1  | Calc.                          |       | 139   |
| Nylon 12-I                                                   |                                         | 18.62                                      | 5.11           | 12.28          | 22.87 |                                |       | 98    |
| Nylon 66                                                     |                                         | 18.62                                      | 0              | 14.12          | 23.37 |                                |       | 56    |
| Nylon 66 (Zytel, DuPont)                                     |                                         |                                            |                |                | 27.8  |                                |       | 118   |
| Poly(iminohexamethylene iminoadipoyl)                        |                                         | 17.43                                      | — 1.92         | 14.89          | 23.02 |                                |       | 56    |
| Poly(amide), thermoplastics (Versamid 930,<br>General Mills) |                                         |                                            |                |                |       |                                |       |       |
| Poly( <i>p</i> -benzamide)                                   |                                         | 18                                         | 11.9           | 7.9            | 23    | Swelling                       |       | 143   |
| Poly( <i>p</i> -phenylene terephthalamide)                   |                                         | 18                                         | 11.9           | 7.9            | 23    | Swelling                       |       | 143   |
| Poly( <i>p</i> -benzanilide terephthalamide)                 |                                         | 18                                         | 11.9           | 7.9            | 23    | Swelling                       |       | 143   |
| Poly( <i>n</i> -isopropyl acrylamide)                        |                                         |                                            |                |                | 22.8  | Calc.                          |       | 154   |
| Gel                                                          |                                         |                                            |                |                | 23.5  | Swelling                       |       | 153   |
| 10.3.2. CELLULOSE AND DERIVATIVES                            |                                         |                                            |                |                |       |                                |       |       |
| Benzyl cellulose                                             |                                         |                                            |                |                | 25.23 |                                |       | 110   |
| Cellulose                                                    |                                         |                                            |                |                | 32.02 |                                |       | 110   |
| Cellulose                                                    |                                         | 12.69                                      | — <sup>a</sup> | 22.3           | 25.66 |                                |       | 81    |
| Cellulose                                                    |                                         | 8.27                                       | 8              | 13.88          | 18.03 |                                |       | 140   |
| Cellulose-alkylketene dimer treatment                        |                                         | 8.1                                        | 12.35          | 7.96           | 16.78 |                                |       | 140   |
| Cellulose acetate (56% acetate groups)                       |                                         |                                            |                |                | 27.83 |                                |       | 110   |
| (48% acetate groups)                                         |                                         |                                            |                |                | 27.19 |                                |       | 110   |
| Cellulose acetate (Cellidore A. Bayer)                       |                                         | 18.6                                       | 12.73          | 11.01          | 25.08 |                                |       | 56    |
| Cellulose acetate                                            |                                         | 15.55                                      | — <sup>a</sup> | 11.87          | 19.56 |                                |       | 81    |
| Cellulose acetate butyrate                                   |                                         | 15.75                                      | — <sup>a</sup> | 8.59           | 17.94 |                                |       | 81    |
| Cellulose acetate propionate                                 |                                         | 15.75                                      | — <sup>a</sup> | 10.23          | 18.76 |                                |       | 18    |
| Cellulose diacetate                                          |                                         |                                            |                |                | 23.22 | Calc.                          |       | 112   |
|                                                              |                                         |                                            |                |                | 22.3  |                                |       | 72    |
|                                                              |                                         |                                            |                |                | 22.3  |                                |       | 110   |
| Cellulose nitrate (11.83% N)                                 |                                         |                                            |                |                | 30.39 |                                |       | 112   |
|                                                              |                                         |                                            |                |                | 21.44 |                                |       | 72    |
|                                                              |                                         |                                            |                |                | 21.7  |                                |       | 21-24 |
|                                                              |                                         |                                            |                |                | 23.5  |                                |       | 72    |
| (11.4% N)                                                    |                                         |                                            |                |                | 21.93 |                                |       | 56    |
| Cellulose nitrate (1/2 sec; H-23 Hagedon)                    |                                         | 15.41                                      | 14.73          | 8.84           | 23.08 |                                |       | 81    |
| Cellulose triacetate                                         |                                         | 15.55                                      | — <sup>a</sup> | 10.64          | 18.84 |                                |       | 81    |
| Cellulose tridecanoate                                       |                                         | 19.85                                      | — <sup>a</sup> | 6.14           | 20.77 |                                |       | 21-24 |
| Ethyl cellulose                                              |                                         |                                            |                |                | 21.1  |                                |       |       |

TABLE 10. cont'd

| Polymer                                                                                     | Molar volume<br>(cm <sup>3</sup> /gmol) | Solubility parameters (MPa) <sup>1/2</sup> |                |                |              | Method              | T(°C) | Refs. |
|---------------------------------------------------------------------------------------------|-----------------------------------------|--------------------------------------------|----------------|----------------|--------------|---------------------|-------|-------|
|                                                                                             |                                         | δ <sub>d</sub>                             | δ <sub>p</sub> | δ <sub>h</sub> | δ            |                     |       |       |
| 10.4. OTHER POLYMERS                                                                        |                                         |                                            |                |                |              |                     |       |       |
| Alcohol soluble resin<br>(Pentalyn 255, Hercules)                                           |                                         | 17.5                                       | 9.3            | 14.3           | 24.4         |                     |       | 56    |
| Alcohol soluble rosin resin<br>(Pentalyn 830, Hercules)                                     |                                         | 20                                         | 5.8            | 10.9           | 23.5         |                     |       | 56    |
| Alkyd, short oil (coconut oil 34% phthalic<br>anhydride, Plexal C34)                        |                                         | 18.5                                       | 9.21           | 4.91           | 21.24        |                     |       | 56    |
| Alkyd resin, medium oil length                                                              |                                         |                                            |                |                | 19.2         |                     |       | 21-24 |
| Alkyd, long oil (66% oil length,<br>Plexal P65, Polyplex)                                   |                                         | 20.42                                      | 3.44           | 4.56           | 12.2         |                     |       | 56    |
| Coumarone-indene resin (Piccoumarone 450L,<br>Penn. Ind. Chem.)                             |                                         | 19.42                                      | 5.48           | 5.77           | 20.99        |                     |       | 56    |
| Epoxy resin                                                                                 |                                         |                                            |                |                | 22.3         |                     |       | 118   |
| Epoxy (Epikote 1001, Shell)                                                                 |                                         | 20.36                                      | 12.03          | 11.48          | 26.29        |                     |       | 56    |
| Epoxy DBEBA-DDMe*                                                                           | 32                                      |                                            |                |                | 22           |                     | 35    | 135   |
| DGEBA-DMM                                                                                   | 22                                      |                                            |                |                | 22.2         |                     | 35    | 135   |
| TGAP-DDMe                                                                                   | 22.4                                    |                                            |                |                | 22.5         |                     | 35    | 135   |
| TGAP-ANI                                                                                    |                                         |                                            |                |                | 23.9         |                     | 35    | 135   |
| TGAP-DDM                                                                                    |                                         |                                            |                |                | 24.8         |                     | 35    | 135   |
| TGAP-DDS                                                                                    |                                         |                                            |                |                | 27.1         |                     | 35    | 135   |
| Ester gum (ester gum BL, Hercules)                                                          |                                         | 19.64                                      | 4.73           | 7.77           | 21.65        |                     |       | 56    |
| Furfuryl alcohol resin (Durez 14383,<br>Hooker Chemical)                                    |                                         | 21.16                                      | 13.56          | 12.81          | 28.21        |                     |       | 56    |
| Hexamethoxymethyl melamine (Cymel 300,<br>American Cyanimid)                                |                                         | 20.36                                      | 8.53           | 10.64          | 24.51        |                     |       | 56    |
| Pentaerythritol ester of rosin, modified<br>(Cellolyn 102, Hercules)                        |                                         | 21.73                                      | 0.94           | 8.53           | 23.37        |                     |       | 56    |
| Petroleum hydrocarbon resin (Piccopale 110,<br>Penn. Ind. Chem.)                            |                                         | 17.55                                      | 1.19           | 3.6            | 17.96        |                     |       | 56    |
| Phenolic resin (resole, Phenodur 373U<br>Chemische Werke Albert)                            |                                         | 19.74                                      | 11.62          | 14.59          | 27.15        |                     |       | 56    |
| Phenolic resin (Super Beckacite 1001,<br>Reichhold)                                         |                                         | 23.26                                      | 6.56           | 8.35           | 25.57        |                     |       | 56    |
| Poly(2-acrylamide-2-methyl propane<br>sulphonamide) (tested in formamide/water<br>mixtures) |                                         |                                            |                |                | 43.6         | Visc.               | 25    | 159   |
| Poly(3,3-dimethyl oxetane)                                                                  |                                         | 15.35                                      | 2.46           | 4.09           | 16.16        | Visc.               |       | 92    |
| Poly(3,3-diethyl oxetane)                                                                   |                                         | 15.55                                      | 2.05           | 3.48           | 16.16        | Visc.               |       | 92    |
| Poly(1,3-dioxolane)                                                                         |                                         |                                            |                |                | 20.66        | Visc.               | 25    | 175   |
| Poly(ether urethane)                                                                        |                                         |                                            |                |                | 17.99 ± 0.02 | IPGC                | 25    | 158   |
|                                                                                             |                                         |                                            |                |                | 17.38 ± 0.16 | IPGC                | 100   | 158   |
|                                                                                             |                                         |                                            |                |                | 17.20 ± 0.15 | IPGC                | 120   | 158   |
|                                                                                             |                                         |                                            |                |                | 17.14 ± 0.14 | IPGC                | 130   | 158   |
|                                                                                             |                                         |                                            |                |                | 17.06 ± 0.15 | IPGC                | 140   | 158   |
|                                                                                             |                                         |                                            |                |                | 16.96 ± 0.15 | IPGC                | 150   | 158   |
| Poly(DL-lactic acid)                                                                        |                                         |                                            |                |                | 21.0 ± 0.3   | Density             | 25    | 142   |
|                                                                                             |                                         |                                            |                |                | 20.5 ± 0.4   | Visc.               | 25    | 142   |
|                                                                                             |                                         |                                            |                |                | 19.8         | Calc. <sup>S</sup>  | 25    | 142   |
|                                                                                             |                                         |                                            |                |                | 20.3         | Calc. <sup>H</sup>  | 25    | 142   |
|                                                                                             |                                         |                                            |                |                | 19.2         | Calc. <sup>HK</sup> | 25    | 142   |
| Poly(oxetane)                                                                               | 17.39                                   |                                            | 5.12           | 5.12           | 19.23        |                     |       | 92    |
| Poly(oxydimethylsilylene)                                                                   |                                         |                                            |                |                | 15.04        |                     |       | 110   |
|                                                                                             |                                         |                                            |                |                | 14.9         | Obs.                |       | 21-24 |
|                                                                                             |                                         |                                            |                |                | 15.45        | Swelling            |       | 76    |
|                                                                                             |                                         |                                            |                |                | 15.6         | Av.                 |       | 76    |
|                                                                                             |                                         |                                            |                |                | 14.9         |                     |       | 118   |
|                                                                                             |                                         |                                            |                |                | 15.59        |                     |       | 45    |
|                                                                                             |                                         |                                            |                |                | 15.4         |                     | 25    | 125   |
|                                                                                             |                                         |                                            |                |                | 15           | Vapor sorp.         |       | 145   |
|                                                                                             |                                         |                                            |                |                | 15.1         | IPGC                |       | 146   |

\* DGEBA - diglycidyl ether of bisphenol A; DDMe - tetraethyl derivative of DDM; DDM - diamino diphenyl methane; TGAP - triglycidyl derivative of amino phenol; ANI - aniline; DDS - diamino diphenylsulfone.

TABLE 10. cont'd

| Polymer                                               | Molar volume<br>(cm <sup>3</sup> /gmol) | Solubility parameters (MPa) <sup>1/2</sup> |                |                |            | Method                  | T(°C) | Refs. |
|-------------------------------------------------------|-----------------------------------------|--------------------------------------------|----------------|----------------|------------|-------------------------|-------|-------|
|                                                       |                                         | δ <sub>d</sub>                             | δ <sub>p</sub> | δ <sub>h</sub> | δ          |                         |       |       |
| δ <sub>2</sub> = (15.7 - 0.026)t, t in °C             |                                         |                                            |                |                | 15.1       | IPGC                    |       | 144   |
|                                                       |                                         |                                            |                |                | 17.5       | <sup>129</sup> Xe shift |       | 152   |
|                                                       |                                         |                                            |                |                | 19.8 ± 2   |                         |       | 157   |
| Poly(ethylene adipate)                                |                                         | 16.3 ± 2                                   | 6.1 ± 0.5      | 9.4 ± 0.1      | 20.2 ± 2   | IPGC                    | 25    | 31    |
| Poly(ethylene oxide)                                  |                                         | 17.3 ± 2                                   | 3.0 ± 1        | 9.4 ± 0.5      | 19.9 ± 2.2 |                         |       | 157   |
|                                                       |                                         |                                            |                |                | 17.8       | Calc.                   |       | 157   |
|                                                       |                                         |                                            |                |                | 19.64      | IPGC                    | 70    | 176   |
|                                                       |                                         |                                            |                |                | 21.9       |                         |       | 118   |
| Poly(oxyethyleneoxyterephthaloyl)                     |                                         |                                            |                |                | 21.9       |                         |       | 112   |
|                                                       |                                         |                                            |                |                | 19.2       | Visc.                   | 25    | 31    |
| Poly(oxytrimethylene) polyoxetane                     |                                         |                                            |                |                | 16.2       | Visc.                   | 25    | 92    |
| -3,3 dimethyl                                         |                                         |                                            |                |                | 16.2       | Visc.                   | 25    | 92    |
| -3,3 diethyl                                          |                                         |                                            |                |                | 16.3       |                         | 81    | 156   |
| Poly(propylene oxide)                                 |                                         |                                            |                |                | 16.2       |                         | 86    | 156   |
|                                                       |                                         |                                            |                |                | 16.1       |                         | 91    | 156   |
|                                                       |                                         | 16.3 ± 1                                   | 4.7 ± 0.5      | 7.4 ± 0.5      | 18.5 ± 1.2 |                         |       | 157   |
|                                                       |                                         |                                            |                |                | 15.9       | Calc.                   |       | 157   |
| Poly(sulfone), Bisphenol A (Udel)                     |                                         | 19.03                                      | 0              | 6.96           | 20.26      |                         |       | 81    |
| Poly(thioethylene)                                    |                                         |                                            |                |                | 19.23      |                         |       | 110   |
|                                                       |                                         |                                            |                |                | 19.19      | Swelling                |       | 43    |
|                                                       |                                         |                                            |                |                | 18.4       | Swelling                |       | 43    |
|                                                       |                                         |                                            |                |                | 19.0 ± 1.0 |                         |       | 87    |
| Poly(thiophenylethylene)                              |                                         |                                            |                |                | 20.5       | Swelling                |       | 76    |
| Poly(urethane) (unknown composition)                  |                                         |                                            |                |                | 20.5       | Av.                     |       | 76    |
|                                                       |                                         |                                            |                |                | 22.9       |                         |       | 155   |
| Poly(urethane), amorphous                             |                                         |                                            |                |                | 16.5       | <sup>129</sup> Xe shift |       | 152   |
| Poly(vinyl ethylene)                                  |                                         |                                            |                |                | 25.6       | Visc.                   |       | 177   |
| Poly(vinyl pyrrolidone)                               |                                         |                                            |                |                | 22.92      | Calc. <sup>HK</sup>     |       | 3     |
| Poly(vinyl methyl ketone)                             | 66.59                                   |                                            |                |                | 22.14      | Calc. <sup>HK</sup>     |       | 3     |
| Poly(vinyl ethyl ketone)                              | 81.58                                   |                                            |                |                | 19.52      | Calc. <sup>HK</sup>     |       | 3     |
| Poly(vinyl methyl sulfide)                            | 66.63                                   |                                            |                |                | 20.28      | Calc. <sup>HK</sup>     |       | 3     |
| Poly(vinyl phenyl sulfide)                            | 118.35                                  |                                            |                |                | 16.72      |                         |       | 56    |
| Terpene resin (Piccolyte S-1000,<br>Penn. Ind. Chem.) |                                         | 16.47                                      | 0.37           | 2.84           |            |                         |       |       |
| Urea-formaldehyde resin (Plastopal H, BASF)           |                                         | 20.81                                      | 8.29           | 12.71          | 25.74      |                         |       | 56    |
| Viton                                                 |                                         | 17                                         | 10.3           | 6.1            | 20.8       |                         |       | 130   |

<sup>a</sup>Altered from previously published value.  
<sup>b</sup>Method of van Krevelen and Hofzyzee.  
<sup>c</sup>Method of Small.  
<sup>d</sup>Method of Hoy.

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# Optically Active Polymers

Katsuhiro Inomata

Department of Polymer Chemistry, Tokyo Institute of Technology, Tokyo, Japan

Akihiro Abe

Department of Industrial Chemistry, Tokyo Institute of Polytechnics, Atsugi, Japan

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|  |         |
|--|---------|
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|--|---------|

C. Optically Active Polymers from Achiral Monomers

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|                                              |         |
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|                        |         |
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By definition the optical activity,  $[M]_D$ , of polymers and their low molecular weight analogs is given by

$$[M]_D = [\alpha]_D \times (\text{mean residue weight})/100$$

## A. ABBREVIATIONS USED

|          |                                                        |
|----------|--------------------------------------------------------|
| AcAc     | Acetylacetone                                          |
| AIBN     | Azobisisobutyronitrile                                 |
| BPO      | Benzoyl peroxide                                       |
| DBP      | Dibenzoyl peroxide                                     |
| DCA      | Dichloroacetic acid                                    |
| DCM      | Dichloromethane                                        |
| DDB      | 2,3-Dimethoxy-1,4-bis(dimethylamino)butane             |
| DMAc     | Dimethylacetamide                                      |
| DMF      | Dimethylformamide                                      |
| DMSO     | Dimethylsulfoxide                                      |
| DPEDA-Li | <i>N,N'</i> -diphenylethylenediamine monolithium amide |
| EDC      | Ethylene dichloride                                    |
| M        | Monomer                                                |
| MC       | Model compound                                         |
| NCA      | <i>N</i> -Carboxylic anhydride                         |
| P        | Polymer                                                |
| RT       | Room temperature                                       |
| TMEDA    | <i>N,N,N',N'</i> -tetramethylethylenediamine           |
| TCA      | Trichloroacetic acid                                   |
| TFA      | Trifluoroacetic acid                                   |
| TFEL     | Trifluoroethanol                                       |
| THF      | Tetrahydrofuran                                        |