Substituting into Equation 2.33 gives:

$$\Delta \bar{H}_{\text{mix},2}\ \alpha\, C_{11} + C_{22} - 2\sqrt{C_{11}C_{22}} = \left(\sqrt{C_{11}} - \sqrt{C_{22}}\right)^2 \tag{2.35}$$

The square roots of the cohesive energy densities are given the designation δ, and have been labeled solubility parameters by Hildebrand (1949); Hildebrand and Scott, (1962). The typical units for this parameter in the early literature were $\sqrt{\text{cal/cm}^3}$, which have been labeled *hildebrands*; the SI unit is the MPa$^{1/2}$ where 1 $\sqrt{\text{cal/cm}^3}$ equals 0.489 MPa$^{1/2}$. Substituting for the square root terms in Equation 2.35:

$$\Delta \bar{H}_{\text{mix},2}\alpha \left(\delta_1 - \delta_2\right)^2 \tag{2.36}$$

The theoretical partial molal enthalpy of mixing resulting from mixing two compounds with different cohesive energy densities was estimated by:

$$\Delta \bar{H}_{\text{mix},2} = \bar{V}_2\phi_1^2\left(\delta_1 - \delta_2\right)^2 \tag{2.37}$$

where ϕ_1 is the fraction of the solution volume occupied by the solvent (Hildebrand and Scott, 1950). For a dilute solution, ϕ_1 is essentially equal to unity.

The cohesive energy density of a pure compound can be estimated by different techniques (Scatchard, 1949; Hoy, 1970; Fedors, 1974). One method (Hildebrand et al., 1970) relates this parameter to the molar enthalpy of vaporization, $\Delta \bar{H}_v$, of the same chemical:

$$C_{22} = \frac{\left(\bar{H}_{v,2} - RT\right)}{\bar{V}_2} \tag{2.38}$$

where $\bar{V}_2$ is the molar volume of the liquid form of the solute in cm^3/mole and $\Delta \bar{H}_v$ is in cal/mole. For liquids that do not have a reported molar enthalpy of vaporization, a convenient method of approximation is Hildebrand's empirical equation, based on the boiling point, T_b, in Kelvin units:

$$\Delta \bar{H}_{v,298\,K} = 0.020T_b^2 + 23.7T_b - 295 \tag{2.39}$$

which yields the molar enthalpy of vaporization in cal/mole (Hildebrand and Scott, 1950). This equation cannot provide an accurate molar enthalpy of vaporization for liquids that are hydrogen bonded. Burrell (1955a, 1955b) found that a final correction can be added to the calculated solubility parameter to provide an estimate reliable enough for most practical applications. One should add 1.4 to the calculated solubility parameter for an alcohol, 0.6 for an ester, and 0.5 for a ketone that boils below 100°C. In other cases, no correction should be necessary.

Substituting Equation 2.37 for the partial molal enthalpy of mixing, along with Equation 2.2 for the partial molal entropy of mixing, which is still considered ideal, and Equation 2.10 for the free energy change in Equation 2.6, gives:

$$RT\ln a_2 = \bar{V}_2\phi_1^2\left(\delta_1 - \delta_2\right)^2 + RT\ln X_2 \tag{2.40}$$

which, from Equation 2.30, tells us that:

$$RT\ln \gamma_2 = \bar{V}_2\phi_1^2\left(\delta_1 - \delta_2\right)^2 \tag{2.41}$$