TABLE 2.1
Fedors Group Contribution Method (1974) Allows Calculation of the Solubility Parameter of Satranidazole

A	B	C	D	E	F
Functional Group or Feature	Number of Times[a]	Cohesive Energy (cal/mole)	Col B*Col C	Contribution to the Molar Volume[b]	Col B*Col E
–CH$_3$	2	1125	2250	33.5	67.0
–CH$_2$–	2	1180	2360	16.1	32.2
=CH–	1	1030	1030	13.5	13.5
=C<	3	1690	5070	6.5	19.5
>N–	3	2800	8400	5.0	15.0
=N–	1	2800	2800	5.0	5.0
–NO$_2$	1	3670	3670	32.0	32.0
–SO$_2$	1	3700	3700	23.8	23.8
Conjugation[c]	2	400	800	–2.2	–4.4
Ring closure	2	250	500	16.0	32.0
Sum			30580		235.6

[a] Indicates number of times that particular functional group or feature appears.
[b] Contribution to the molar volume by the particular functional group or feature.
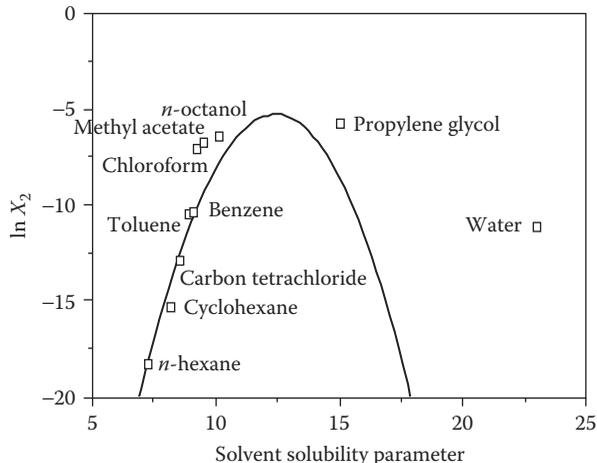[c] Conjugation indicates a series of double then single then double then single bonds.

FIGURE 2.3   Regular solution theory plot for hydrocortisone solubility data. The curve presents the solubility predicted by Equation 2.43 using data from *n*-hexane, cyclohexane, carbon tetrachloride, toluene, and benzene to estimate the solubility parameter of hydrocortisone. (Data from Hagen, T. A., Physicochemical study of hydrocortisone and hydrocortisone n-alkyl-21-esters, PhD dissertation, University of Michigan, pp. 94–96, 1979. With permission.)

n-heptane ($\delta_1 = 7.50$), the solute solubility parameter for each para-aminobenzoate studied could be easily estimated using Equation 2.43 and the solubility in that nonpolar solvent (Neau et al., 1989). The solubility data associated with the nonpolar solvents is regressed as a quadratic equation in the solvent solubility parameter, acknowledging that the enthalpy of fusion term on the right-hand side of Equation 2.43 is a constant under these conditions, to estimate the solute solubility parameter.