Chapter 14

SOLUBILITY PARAMETER, LIQUID VOLUME AND VAN DER WAALS AREA AND VOLUME

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ABSTRACT

Results for solubility parameter, liquid volume and Van der Waals area and volume are presented for major organic and inorganic chemicals. The chemical formula and molecular weight are also given. The results are displayed in easy-to-use tabulations that are especially applicable for rapid engineering usage with the personal computer or hand calculator.

INTRODUCTION

Properties such as solubility parameter and liquid volume are useful in modeling of phase equilibrium in the chemical processing and petroleum refining industries. As an example of such usefulness in vapor-liquid operations, calculation of activity coefficients using regular solution methods for phase equilibrium in distillation, stripping and absorption requires knowledge of solubility parameter and liquid volume for the species in the mixture.

SOLUBILITY PARAMETER AND LIQUID VOLUME

The results for solubility parameter and liquid volume are given in Tables 14-1 and 14-2 for organic and inorganic compounds. The values for solubility parameter are ascertained from data for heat of vaporization and liquid volume (molecular weight/density): $[(Hvap - RT)/v]^{0.5}$. For compounds that are liquids at ambient conditions, the values apply at 25 C. For compounds that are gases at ambient conditions, the values apply at the normal boiling point temperature. For compounds that are solids at ambient conditions, the values apply at the melting point temperature. The tabulations are based on data source publications for organics (1-40) and inorganics (1-120). The tabulations are arranged by chemical formula to provide ease of use in quickly locating data.

VAN DER WAALS AREA AND VOLUME

The results for Van der Waals area and volume are also given in Tables 14-1 and 14-2 for organic and inorganic compounds. The tabulations are based on data source publications for organics (1-5) and inorganics (1-5). Van der Waals area and volume involve the surface area and volume of an atom and maybe ascertained from bond distances, contact distances and shapes of atoms. Methods of calculation are described by Bondi (2).

REFERENCES - SOLUBILITY PARAMETER AND LIQUID VOLUME - ORGANIC COMPOUNDS

1-34. See **REFERENCES - ORGANIC COMPOUNDS** in **Chapter 5 ENTHALPY OF VAPORIZATION**
35-40. See **REFERENCES - ORGANIC COMPOUNDS** in **Chapter 8 DENSITY OF LIQUID**

REFERENCES - SOLUBILITY PARAMETER AND LIQUID VOLUME - INORGANIC COMPOUNDS

1-56. See **REFERENCES - INORGANIC COMPOUNDS** in **Chapter 5 ENTHALPY OF VAPORIZATION**
57-120. See **REFERENCES - INORGANIC COMPOUNDS** in **Chapter 8 DENSITY OF LIQUID**

REFERENCES - VAN DER WAALS AREA AND VOLUME - ORGANIC COMPOUNDS

1. Daubert, T. E. and R. P. Danner, DATA COMPILATION OF PROPERTIES OF PURE COMPOUNDS, Parts 1, 2, 3 and 4, Supplements 1 and 2, DIPPR Project, AIChE, New York, NY (1985-1992).
2. Bondi, A., PHYSICAL PROPERTIES OF MOLECULAR CRYSTALS, LIQUIDS AND GLASSES, John Wiley and Sons, Inc., New York, NY (1968).
3. Bondi, A., J. Phys. Chem., 68, 441 (1964).
4. Edward, J. T., J. Chem. Educ., 47, 261 (1970).
5. Vera, J. H., S. G. Sayegh and G. A. Ratcliff, Fluid Phase Equilibria, 1, 113 (1977).

REFERENCES - VAN DER WAALS AREA AND VOLUME - INORGANIC COMPOUNDS

1-5. See above **REFERENCES - VAN DER WAALS AREA AND VOLUME - ORGANIC COMPOUNDS**