ESTIMATION OF THE DENSITIES OF TRIGLYCERIDE AND ALCOHOL SOLUTIONS IN THE 278 - 313 K RANGE

M. RODRIGUEZ RODRIGUEZ AND M. GALAN VALLEJO

Department of Chemical Engineering, University of Cádiz, Apdo 40, Puerto Real 11510 (Cádiz), Spain

Recibido el 13 de abril de 1994

En versión definitiva el 5 de septiembre de 1994

RESUMEN.- Se propone una ecuación para estimar el valor de la densidad de disoluciones de triglicéridos y alcoholes (triacetina-butanol, tributirina-butanol, tricaprilina-butanol, tributirina-etanol y tributirina-hexanol), cuyos parámetros se calculan a partir de la densidad y masa molecular de los componentes puros, en el intervalo de temperatura de 278 a 313 K, siendo el porcentaje de desviación media absoluta del 1.3% en el caso más desfavorable.

SUMMARY.- An equation is proposed for estimating the value of the density of triglyceride and alcohol solutions (triacetin-butanol, tributyrin-butanol, tricaprylin-butanol, tributyrin-ethanol and tributyrin-hexanol) whose parameters are calculated from the density and molecular mass of the pure components, in the 278 -313 K temperature range, with a worst-case absolute average deviation of 1.3%.

Key words: Density, triglyceride, alcohol, solution.

INTRODUCTION

The study of the physico-chemical behavior of liquids needs the knowledge of pure component properties and their mixtures. These mixtures properties depend on their composition and molecular structure of the components. Theoretical study is hard due to the complexity of the liquid state, and most of the actual treatments for predicting these properties are empiricals or semiempirical.

The liquid state has analyzed with models similar to gas state or solid state, the former including the radial distribution theories, and the later considering reticular theories. However, none of them has been successful in the production of equations and relation ships for prediting the properties of pure liquids and mixtures.

The interest in knowing the density of liquids and their mixtures is due not just to their involvement in chemical engineering design calculations but also in the study of mixture excess properties. Frequently, these properties are required for conditons at which no data exist and numerous correlations have there fore appeared in the literature.

Most methods for estimating the density of liquids and their mixtures are based on the law of corresponding states, knowledge of critical properties, or group contributions. There are various models for predicting the density of saturated liquids as a function of temperature using the law of corresponding states (1)(2), or of liquid mixtures (3)(4) or using group contributions for amorphous polymers (5), for liquids at 25°C (6), and for solvents, oligomers and polymers (7).

The equation proposed may constitute a simple method for estimating the density of solutions of molecular compounds similar to those employed.

PROPOSED EQUATION

The proposed equation relates the solution's density to the composition and temperature as follows:

$$\ln\left(\frac{1}{\rho}\right) = \frac{a}{M} + b\,T + c \qquad [1]$$

where " ρ " is the density of the solution, "M" the value of the average molecular weight, "T" the temperature absolute and "a", "b" and "c" are parameters of equation.

DISCUSSION AND CONCLUSION

Parameters a, b and c were calculated from the experimental density data (8), their values are ser out on Talbe I, with reference temperatures 278 and 313 K.

The absolute average deviation (AAD) between the

density values estimated using equation [1] and the experimental values are set out on Table I. In most cases, the average deviation is less than 1%; this is exceeded only in the triacetion-butanol system. The results show that the proposed equation does, within the temperature range considered, satisfactorily predict the density values of the triglyceride and alcohol solutions used, for the whole range of composition.

TABLA I

Parameters of equation (1)

Solutions	a	b	c	AAD(%)
Triacetin-butanol	40.2	9.7×10^{-4}	- 0.616	1.30
Tributyrin-butanol	23.7	9.7×10^{-4}	- 0.394	0.52
Tricaprylin-butanol	14.2	9.7×10^{-4}	- 0.266	0.25
Tributyrin-ethanol	14.4	11.2×10^{-4}	- 0.407	0.65
Tributyrin-hexanol	35.9	8.9×10^{-4}	- 0.414	0.87

Absolute average deviation percentage is calculated as: $AAD = 100 \times 1/n \Sigma [(\rho_{calc} - \rho_{exp})/\rho_{exp}]$ where n is number of points for each solutions.

Equation [1] represents an adequate empirical method for estimating the densities of this type of solution, without the need to include parameters revealing the existence of inter-molecular interactions which are an added difficulty, the procedures for their calculation being bothersome. The method is extremely simple to use and is suitable for design applications.

REFERENCES

1. RACKETT, H.G.; Equation of State for Satured Liquids. *J. Chem. Eng. Data,* **15**, 514 (1970).
2. BHIRUD, V.S.; Satured Liquid Densities of Normal Fluids. *AIChE J.,* **24**, 1127 (1978).
3. TEJA, A.S., RICE, P.A.; Multifluid Corresponding States Principle for the Thermodynamic Properties of Fluid Mixtures. *Chem. Eng. Sci.,* **36**, 1 (1981).
4. RICE, P., TEJA, A.S.; The Measurement and Prediction of the Densities of the Rernary Mixtures Hexane + Hexadecane + n-Propyl Alcohol. *Chem. Eng. Sci.,* **37**, 1675 (1982).
5. VAN KREVELEN, D.W., HOFTYZER, P.J.; *Properties of Polymers. Correlation with Chemical Structure.* Esevier Scientific, Chapter 4, pp 41-65, Amsterdam (1972).
6. FEDORS, R.F.; A Method for Estimating Both the Solubility Parameter and Molar Volumes of Liquids. *Polym. Eng. Sci.,* **14**, 147 (1974).
7. ELBRO, H.S., FREDESLUND, A., RASMUSSEN, P.; Group Contribution Method fot the Prediction of Liquid Densities as a Function of Temperature for Solvents, Oligomers and Polymers. *Ind. Eng. Chem. Res.,* **30**, 2576 (1991).
8. RODRIGUEZ, M., GALAN, M., MUÑOZ, Mª.J., MARTIN, R.; Viscosity of Triglycerides + Alcohols from 278 to 313 K. *J. Chem Eng. Data.* **39**, 102 (1994).