Transport, optical thermodynamic and an interfacial (surface tension) property have been computed for three binary and one ternary system (2-propanol + tetrahydrofuran + 2,2,4 trimethylpentane and its constituent binaries) at 4 different temperatures ranging between 298.15 and 323.15 K. Viscosity, the most important transport property, having vast significance in industrial applications especially design calculations, has been computed by employing more than 10 approaches. These include empirical, semi-empirical, correlative and predictive methods. Refractive index, an optical and transport property of importance has also been computed by using 10 approaches. A new approach has been put to test for computing the refractive index for binary systems and has been extended for ternary system under investigation. Surface Tension, an interfacial property has also been computed. Further, excess Gibbs free energy of activation of viscous flow ($\Delta G^*$) has also been elucidated to predict the nature of interactions for all the four systems to get a better understanding of the various intermolecular interactions taking place thereof. The results obtained are compared with the experimental findings taken from literature and a comparative study has been carried out regarding the merit/demerits of the various approaches used for the present investigation. Good agreement with the experimental data is observed. An attempt will also be made to compute thermodynamic properties from literature data.

References