The solubility of drugs were measured in 6 alkanols (ethanol, 1-propanol, 1-butanol, 1-pentanol, 1-hexanol, 1-heptanol) at temperature ranging from 278.15 to 318.15 K. Before starting the experiment, to check the miscibility of drugs in solvents, molecular dynamics (MD) simulations were performed using the COMPASS force field, and the cohesive energy density and solubility parameters were determined for the model compounds. According to previous studies, the difference of solubility parameter is greater than 10.0 is indicative of an immiscible system. It was confirmed that all solvents and drugs are miscible systems. After experimenting, activity coefficient approaches were used for correlation of drugs. Activity coefficients for solubilities of drugs in alkanols have been calculated by means of the NRTL, UNIQUAC and Wilson equations and were correlated with solubility data that were compared with the experimental ones. All three correlation results are in good agreement with the experimental data. The quasi-chemical nonrandom lattice fluid theory (QLF) equation of state (EOS) were also applied to calculating solubilities of drugs in alkanols.