The binary phase diagram studies of the thermal energy storage materials (organic crystalline materials) have been performed by using high temperature X-ray diffraction characterization and differential scanning calorimetric (DSC) methods. Thermal energy storage materials undergo a solid-solid phase transition before melting which will store large amounts of thermal energy. Three materials [tris(hydroxymethyl)aminomethane (TRIS) and 2-Amino-2-methyl-1, 3-propanediol (AMPL) and Pentaglycerol (PG)] were used for this study. The binary AMPL-TRIS and AMPL-PG phase diagrams have been developed. The high temperature solid-state phases of AMPL and TRIS were characterized as a disordered BCC structure, and PG was characterized as FCC. Lattice and volume expansion calculations on single phase of AMPL, TRIS and PG have been performed. Calculation of Phase Diagrams (CALPHAD) modeling technique is used to calculate the AMPL-TRIS and AMPL-PG binary phase diagrams by using the Thermal-Calc software. The detail of the thermal properties and excess Gibbs energies will present.