عنوان مقاله:

An experimental and computational investigation of the mixtures of morpholine and propylene glycol

محل انتشار:

سومین کنفرانس بین المللی علوم پایه و علوم مهندسی (سال: 1400)

تعداد صفحات اصل مقاله: 5

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خلاصه مقاله:

The thermodynamic properties for the binary mixtures of morpholine and propylene glycol have been measured at temperature ۲۹۸.۱۵ K and at atmospheric pressure. From the data of measured densities, the excess molar volumes have been calculated. Additionally, the molecular dynamics (MD) simulation technique was used to compute the densities, radial distribution functions (RDFs) and mean square displacement (MSD) of the mixtures with different mole fractions at ۲۹۸.۱۵ K and at ۱ atm. Also, the hydrogen bonding interactions were investigated by MD and quantum calculations.

کلمات کلیدی:

Density, DFT, Molecular dynamic simulation

لینک ثابت مقاله در پایگاه سیویلیکا: