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Preferential Solvation of Ethylhexyl Triazone in Ethyl Acetate + EtOH Mixtures According to the Inverse Kirkwood-Buff Integrals Method

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***SUMMARY*. The preferential solvation parameters, that is, the differences between the local and bulk mole fractions of the solvents in solutions of the sunscreen compound ethylhexyl triazone (EHT) in ethyl acetate (EtAc) + ethanol (EtOH) binary mixtures are derived from their thermodynamic properties by means of the inverse Kirkwood-Buff integrals (IKBI) method. From solvent effect studies, it is found that EHT is sensitive to solvation effects, so the preferential solvation parameter $\delta x_{EtAc,EHT}$, is negative in ethanol-rich and ethyl acetate-rich mixtures but positive in compositions from 0.36 to 0.71 in mole fraction of AcEt at 298.15 K. It is conjecturable that in EtOH-rich mixtures the interaction by acidic hydrogen-bonding by EtOH on basic sites of the sunscreen compound plays a relevant role in the solvation. The more solvation by AcEt in mixtures of similar solvent compositions could be due mainly to polarity effects. Finally, the slight preference of this compound for EtOH in AcEt-rich mixtures could be explained in terms of the common participation of basic sites in both solvents and/or the acidic site of EtOH with the respective counterparts of ethylhexyl triazone. Nevertheless, the specific solute-solvent interactions remain unclear.**

KEY WORDS: Ethylhexyl triazone, Ethanol, Ethyl acetate, Inverse Kirkwood-Buff integrals, IKBI, Preferential solvation.

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