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Solvent effect on the volume of the DielsAlder reaction between tetracyanoethylene and trans,trans-1,4-diphenyl-1,3-butadiene

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Abstract

From the partial molar volumes of tetracyanoethylene, trans,trans-1,4-diphenyl-1,3-butadiene, and their Diels-Alder adduct, the volumes of the reaction in a series of solvents at 25°C (cm³ mol⁻¹) were calculated: in dioxane, -26.4; in chloroform, -34.9; in ethyl acetate, -34.5; in acetonitrile, -4.4; in cyclohexanone, -34.0; in 1,2-dichloroethane, -31.8; in benzene, -26.9; in toluene, -24.5; in o-xylene, -21.1; and in mesitylene, -16.9. The solvent effects on the activation and reaction volumes and on the partial molar volumes of the reactants, activated complex, and adduct were discussed.

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