

Ene reaction between 4-phenyl-1,2,4-triazoline-3,5-dione and hex-1-ene. The enthalpies, entropies, and volumes of activation and reaction in solution

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Abstract

The rates of an ene reaction between 4-phenyl-1,2,4-triazoline-3,5-dione and hex-1-ene were studied in a temperature range of 15-40 °C and in a pressure range of 1-2013 bar. The enthalpy of reaction in 1,2-dichloroethane (-158.2 ± 1.0 kJ mol⁻¹), the enthalpy (51.3 ± 0.5 kJ mol⁻¹), entropy (122 ± 2 J mol⁻¹ K⁻¹), and volume of activation (-31.0 ± 1.0 cm³ mol⁻¹), and the volume of this reaction (-26.6 ± 0.3 cm³ mol⁻¹) were determined. The high exothermic effect of the reaction suggests its irreversibility. © 2014 Springer Science+Business Media, Inc.

<http://dx.doi.org/10.1007/s11172-014-0424-y>

Keywords

4-phenyl-1,2,4-triazoline-3,5-dione, Ene reaction, Hex-1-ene, High pressure, Kinetics, Thermochemistry