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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

Kiselev V., Kashaeva H., Potapova L., Kornilov D., Konovalov A.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

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.

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Keywords

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