

heat capacity of activation, $\Delta^\ddagger C_p^\circ$

A quantity related to the temperature coefficient of $\Delta^\ddagger H$ (enthalpy of activation) and $\Delta^\ddagger S$ (entropy of activation) according to the equations:

$$\Delta^\ddagger C_p = \left(\frac{\partial \Delta^\ddagger H}{\partial T} \right)_p = T \left(\frac{\partial \Delta^\ddagger S}{\partial T} \right)_p$$

If the rate constant is expressible in the form

$$\ln k = \frac{a}{T} + b + c \ln T + dT,$$

then:

$$\Delta^\ddagger C_p = (c - 1) R + 2 d(R T)$$

SI unit: J mol⁻¹ K⁻¹.

Source:

PAC, 1994, 66, 1077 (*Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994)*) on page 1120

PAC, 1996, 68, 149 (*A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996)*) on page 168