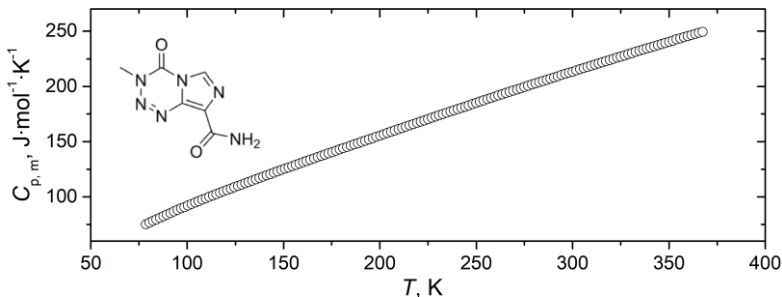


## Thermodynamic parameters of temozolomide

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Temozolomide is an orally administered alkylating agent, which causes DNA damage leading to tumor cell death, and it is used largely in the therapy of glioblastoma [1]. The results of complex thermodynamic study of temozolomide are represented in this work. The sample contained 99.6 mas. % of the compound. Heat capacities of temozolomide in crystalline state at saturation pressure in the range of (80 – 370) K (Fig) were determined in TAU-10 vacuum adiabatic calorimeter [2]. Relative expanded uncertainty of the heat capacity measurements was determined to be 0.4 %. Standard thermodynamic functions of the compound in condensed state in range of (80 and 370) K were calculated from the received data and the values of heat capacity, entropy, reduced enthalpy and Gibbs energy at  $T = 298.15$  K were determined to be  $(212.3 \pm 0.8)$ ,  $(175.4 \pm 0.7)$ ,  $(108.1 \pm 0.4)$  and  $-(67.29 \pm 0.82)$  J mol<sup>-1</sup> K<sup>-1</sup> respectively. Standard thermodynamic functions of temozolomide in gaseous state in the range of (0 – 1500) K were calculated using statis



**Fig.** The heat capacities of crystalline temozolomide

Standard combustion energy of crystalline temozolomide at 298.15 K was determined in a combustion calorimeter B-08-MA [2]. Standard enthalpies of combustion and formation of crystalline temozolomide at 298.15 K were obtained to be  $\Delta_c H^\circ = -(3154.46 \pm 0.56)$  kJ·mol<sup>-1</sup> and  $\Delta_f H^\circ = -(64.11 \pm 0.97)$  kJ·mol<sup>-1</sup>. The method of isodesmic reactions was proposed to calculate the gas-phase formation enthalpies of temozolomide. Sublimation enthalpy was calculated in the framework of electrostatic potential model.

### References

- [1] T.C. Carter et al. BioMed Research International (2018) 1.
- [2] G. J. Kabo et al. J. Chem. Thermodyn. (2019) 225.