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Vapor pressures and vaporization enthalpies of 5-nonanone, linalool and 6-methyl-5-hepten-2-one. Data evaluation

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ABSTRACT

Vapor pressures and vaporization enthalpies for 5-nonanone, linalool and 6-methyl-5-hepten-2-one seem to be in disarray. Temperature dependences of vapor pressures for these pure compounds were measured by using the static and the transpiration techniques. Molar standard enthalpies of vaporization at the reference temperature were derived. Available literature data on vapor pressures and vaporization enthalpies were collected and analyzed. The consistent data set for each compound was evaluated. Reliable thermodynamic parameters of vaporization were derived and used to test some commonly used predicting procedures.

1. Introduction

This work has been inspired by a paper published in this journal recently [1]. This paper presented a descriptor based group contribution model for the prediction of the vaporization enthalpies of organic compounds. The database used in this work consisted of 4320 experimental data points for 2811 compounds. The authors used single experimental values available for 2049 compounds. For the remaining 762 compounds, the arithmetic average was used where multiple values were available. The authors explicitly noted that no attempt was made to choose between the independently determined values, which for the most part differed by less than 9 kJ mol^{-1}. The exceptions to this were made for 30 compounds presented in their Table 1, where experimental vaporization enthalpies have shown the spread of values more than 9 kJ mol^{-1}. To our surprise in this table we have revealed 13 compounds, which have been carefully evaluated in our lab over the last decade. Under evaluation we understand additional experiments, uniform treatment of the available literature data, consistency tests and final recommendation of the evaluated data sets for parent group of compounds. The presented work is intended as the assistance to the community dealing with structure–property relationships, similar to the one hereby reported [1].

In order to avoid an any misunderstandings, that the aforementioned 13 compounds still need revision of the vapor pressure data we provide a list with these compounds and references as follows: *cis*-1,2-diphenylethylene [2], 1-methylimidazole [3], pyrimidine [4], 1,2-propanediol [5], triethylenetetramine and ethylenediamine [6], formamide [7], *N*-(2-hydroxyethyl) ethylenediamine [8], butyl formate [9], 4-chloroaniline [10], propylene carbonate [11], diethyl oxalate [12], and benzyl alcohol [13]. In any case, any indication of unreliable data suggested by Ref. [1] is valuable advice and identifies questionable compounds that should be remeasured.

In the current study we have been guided by the paper by Gharagheizi et al. [1] and have measured vaporization enthalpies of 5-nonanone and (±)-linalool claimed as unreliable. In addition to that we have studied 6-methyl-5-hepten-2-one whose vaporization enthalpy was available only at high temperatures [14,15].

The aliphatic ketone 5-nonanone is used as industrial solvent and also used as platform chemical for production of liquid hydrocarbon fuels (diesel and gasoline) [16]. The aliphatic alcohol (±)-linalool has wide application as perfume, pesticide, and insecticide component [17]. Just recently, the allergic reaction caused by oxidation of linalool to 6-methyl-5-hepten-2-one has been observed [18]. Moreover, the 6-methyl-5-hepten-2-one is also used in household and hygiene products like cleaning agents and air fresheners [19]. Thus, this compound is involved in oxidation reactions resulting in products responsible for possible adverse health effects in the eyes and airways [19].

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