CHEMICAL DATABASES AS A PROMISING TOOL FOR OBTAINING THE VAPORIZATION CHARACTERISTICS OF ORGANIC COMPOUNDS

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Understanding the thermodynamic properties of vaporization for organic compounds is necessary for industrial applications such as separation, synthesis and for developing theoretical models of intermolecular forces and solubility. Despite there being over 20 million known organic compounds, thermodynamic data exists for only about 0.1% of them. This fact is due to the substantial time and resources required for experimental measurement of saturated vapor pressures and vaporization enthalpy.

Chemical databases like Reaxys and SciFinder hold a large number of boiling point data (usually collected during substance identification in synthesis studies); these values often contain significant errors due to equipment limitations or sample impurity. Consequently, thermodynamics specialists have rarely used this data.

This study presents a methodology to process such existing data to model the temperature dependence of saturated vapor pressure in a wide range. Testing on five reference compounds showed that the method determines vapor pressure with up to 20% error and vaporization enthalpy with up to 2.0 kJ/mol error, which is comparable with the precision of many experimental techniques [1].

The procedure was successfully applied to over 100 compounds, yielding vapor pressure and enthalpy dependencies. For several substances, this data is novel; for others, it corroborates existing literature or helps resolve discrepancies through critical analysis [2]. Given the sheer volume of data in chemical databases, this approach can be scaled to analyze thousands of substances lacking high-precision studies and serves as a tool for validating uncertain literature values.

1. Nizamov I. I., Bolmatenkov D. N., Yagofarov M. I., Solomonov B. N. // J. Mol. Liq. 2025. Vol. 417, Article ID 126645. https://doi.org/10.1016/j.molliq.2024.126645

2. Bolmatenkov D. N., Nizamov I. I., Solomonov B. N., Yagofarov M. I. // JCED 2025. Vol. 70(11), P. 4351-4361. https://doi.org/10.1021/acs.jced.5c00506

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