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Understanding the thermodynamic properties of substances like toluene is crucial in fields such as chemical engineering, physical chemistry, and material science. Among these properties, the heat of vaporization (H) and entropy change (S) during phase transitions are fundamental parameters that describe how a substance behaves under different conditions. In this article, we will explore how to calculate the change in entropy (ΔS) during the vaporization of toluene, given its heat of vaporization of 38.1 kJ/mol. We will delve into the underlying principles, detailed calculations, and implications of this thermodynamic process.

Introduction to Vaporization and Entropy

Vaporization is the phase transition where a substance changes from a liquid to a gas. This process can occur through boiling or evaporation, depending on the conditions. It involves an energy input to overcome intermolecular forces, leading to the molecules escaping into the vapor phase.

Entropy (S) is a thermodynamic property that measures the degree of disorder or randomness in a system. During vaporization, the entropy of the system increases because the molecules become more disordered as they transition from a structured liquid to a more dispersed gaseous state.

The change in entropy during vaporization (ΔS) at a specific temperature is closely related to the heat of vaporization (H) and can be approximated using thermodynamic principles. This relationship provides insights into the spontaneity of phase changes and the energy requirements involved.

Fundamental Relationship Between Heat of Vaporization and Entropy

The calculation of entropy change during vaporization relies primarily on the fundamental thermodynamic relationship:

Clausius Equation

$$\Delta S_{\text{vap}} = \frac{\Delta H_{\text{vap}}}{T}$$

Where:

- ΔS_{vap} is the entropy change during vaporization (J/K·mol),
- ΔH_{vap} is the heat of vaporization (J/mol),
- T is the temperature at which vaporization occurs (Kelvin).

This equation assumes that the heat of vaporization remains constant over the temperature range and that vaporization occurs at equilibrium.

Given Data for Toluene

Before performing any calculations, let's review the provided data:

- Heat of vaporization, $\Delta H_{\text{vap}} = 38.1 \text{ kJ/mol}$
- Temperature of vaporization, $T_b \approx 110.6^\circ\text{C}$ or 383.7 K (boiling point of toluene at 1 atm)

Note: The boiling point temperature of toluene at standard atmospheric pressure (1 atm) is approximately 110.6°C. This temperature is where vaporization occurs at equilibrium under standard conditions.

Calculating the Change in Entropy (ΔS) for Toluene Vaporization

Using the Clausius equation, the entropy change during vaporization at the boiling point can be calculated as follows:

$$\Delta S_{\text{vap}} = \frac{\Delta H_{\text{vap}}}{T}$$

Convert ΔH_{vap} into Joules:

$$\Delta H_{\text{vap}} = 38.1 \text{ kJ/mol} = 38,100 \text{ J/mol}$$

Temperature in Kelvin:

$$T = 110.6^{\circ}\text{C} + 273.15 = 383.75\text{ K}$$

Now, substitute into the equation:

$$\Delta S_{\text{vap}} = \frac{38,100\text{ J/mol}}{383.75\text{ K}} \approx 99.2\text{ J/K}\cdot\text{mol}$$

Result:

$$\boxed{\Delta S_{\text{vap}} \approx 99.2\text{ J/K}\cdot\text{mol}}$$

This value indicates the increase in entropy when one mole of toluene vaporizes at its boiling point under atmospheric pressure.

Interpreting the Results and Thermodynamic Significance

The calculated entropy change provides valuable insights:

1. Spontaneity of Vaporization:

Since ΔH_{vap} is positive (endothermic), and ΔS_{vap} is also positive, the vaporization process is thermodynamically favorable at temperatures above the boiling point when the Gibbs free energy change ΔG is negative.

2. Temperature Dependence:

The entropy change during vaporization remains approximately constant near the boiling point, but at different temperatures, the actual value may vary slightly due to non-ideal behavior.

3. Relation to Vapor Pressure:

The entropy change relates to the vapor pressure of toluene and can be used to estimate how the vapor pressure varies with temperature, applying the Clausius-Clapeyron equation.

Extending the Calculation to Other Temperatures

While our calculation focuses on vaporization at the boiling point, the entropy change can be extended to other temperatures using the integrated Clausius-Clapeyron relation:

$$\ln P = -\frac{\Delta H_{\text{vap}}}{RT} + C$$

Where:

- P is vapor pressure,
- R is the universal gas constant (8.314 J/mol·K),
- C is a constant.

This relation indicates that the entropy change per mole during vaporization is approximately constant for small temperature ranges, but precise calculations should account for temperature dependence.

Practical Applications and Implications

Understanding the entropy change during vaporization has several practical applications:

- **Design of Chemical Processes:** Engineers can optimize distillation and separation processes by understanding the thermodynamics of toluene vaporization.
- **Thermodynamic Modeling:** Accurate entropy values improve models predicting phase equilibria and vapor-liquid equilibria (VLE).
- **Environmental and Safety Considerations:** Knowledge of vaporization properties informs safety protocols when handling volatile organic compounds like toluene.
- **Material Compatibility:** Knowing the thermodynamic properties helps in selecting appropriate materials resistant to toluene's vapor phase.

Summary and Key Takeaways

- The heat of vaporization of toluene at its boiling point is 38.1 kJ/mol.
- Using the Clausius equation, the change in entropy during vaporization at the boiling point is approximately 99.2 J/K·mol.
- This entropy increase reflects the greater disorder as toluene transitions from liquid to vapor.
- The thermodynamic insights gained assist in process design, safety, and environmental considerations involving toluene.

Additional Considerations and Advanced Topics

While the basic calculation provides a solid understanding, more advanced analyses may involve:

1. **Non-Ideal Behavior:** Considering deviations from ideality using activity coefficients and fugacity.
2. **Temperature Dependence of H :** Accounting for changes in heat of vaporization with temperature, often modeled using empirical correlations.
3. **Entropy of Condensation:** The reverse process, where vapor condenses into liquid, involves a decrease in entropy of the same magnitude.
4. **Thermodynamic Cycles:** Applying these properties within refrigeration cycles or heat engines involving toluene as a working fluid.

Conclusion

Calculating the change in entropy during vaporization is a fundamental aspect of thermodynamics that enhances our understanding of phase transitions in chemical substances like toluene. The relationship between heat of vaporization and entropy change, governed by the Clausius equation, provides a straightforward method for quantifying the disorder introduced during vaporization. This knowledge is essential in designing chemical processes, ensuring safety, and optimizing industrial applications involving volatile organic compounds.

Remember: Always consider the specific conditions and potential deviations from ideality when applying these calculations in real-world scenarios. Accurate thermodynamic data and models lead to better process control and safer handling of chemicals like toluene.

Frequently Asked Questions

What is the heat of vaporization (H) of toluene in kJ/mol?

The heat of vaporization (H) of toluene is 38.1 kJ/mol.

How do you calculate the change in entropy (ΔS) when

toluene vaporizes?

The change in entropy can be calculated using the formula $\Delta S = H/T$, where H is the heat of vaporization and T is the temperature in Kelvin.

At what temperature should the entropy change be calculated for toluene vaporization?

Typically, the entropy change is calculated at the boiling point of toluene, which is approximately 110.6°C or 383.75 K.

What is the formula to find ΔS when given H and T?

The formula is $\Delta S = H / T$, with H in joules and T in Kelvin, to get the entropy change in J/K·mol.

Convert the heat of vaporization of toluene from kJ/mol to J/mol.

38.1 kJ/mol equals 38100 J/mol.

Calculate the change in entropy (ΔS) for toluene vaporization at its boiling point.

Using $\Delta S = H / T$, $\Delta S = 38100 \text{ J/mol} / 383.75 \text{ K} \approx 99.2 \text{ J/K}\cdot\text{mol}$.

Why is understanding the entropy change important in thermodynamics?

It helps in predicting the spontaneity of phase changes and understanding energy dispersal during vaporization.

Can the entropy change for toluene vaporization be negative?

No, the entropy change for vaporization is positive because the disorder increases when a liquid turns into vapor.

Additional Resources

The Heat of Vaporization (H) of Toluene ($\text{C}_6\text{H}_5\text{CH}_3$) Is 38.1 kJ/mol. Calculate the Change in Entropy (S) When

Introduction: Understanding the Significance of Vaporization and Entropy in Thermodynamics

In the realm of physical chemistry, thermodynamics provides a foundation for deciphering the energetic and molecular transformations that substances undergo during phase changes. Among these fundamental concepts are the heat of vaporization (H) and entropy (S), both pivotal in understanding the molecular dynamics during boiling, condensation, and other phase transitions.

The heat of vaporization (H) refers to the amount of energy required to convert one mole of a liquid into vapor at constant temperature and pressure, overcoming intermolecular forces. For toluene ($\text{C}_6\text{H}_5\text{CH}_3$), a widely used solvent in chemical industries and laboratories, this value is given as 38.1 kJ/mol.

Entropy (S), on the other hand, is a measure of the disorder or randomness within a system. During vaporization, the transition from a more ordered liquid phase to a less ordered gaseous phase involves a significant increase in entropy.

This article delves into the thermodynamic principles linking the heat of vaporization to entropy change, providing a comprehensive analysis and step-by-step calculation of the change in entropy (ΔS) for toluene vaporization. Such understanding not only enriches theoretical knowledge but also has practical implications in chemical engineering, environmental science, and industrial processes.

Fundamentals of Vaporization and Thermodynamic Relationships

What Is the Heat of Vaporization?

The heat of vaporization (H) quantifies the energy needed to convert a liquid into vapor at constant pressure (usually atmospheric). It reflects the energy required to overcome the intermolecular forces — such as London dispersion, dipole-dipole interactions, and hydrogen bonding — that hold molecules in the liquid phase.

Key points about H :

- Units: Typically expressed in joules per mole (J/mol) or kilojoules per mole (kJ/mol).
- Temperature Dependence: H generally decreases with increasing temperature as molecules gain kinetic energy.
- Relevance: Critical in designing distillation processes, understanding climate phenomena, and calculating phase equilibria.

Entropy and Its Role in Phase Changes

Entropy (S) measures the degree of disorder or randomness. When a substance vaporizes, molecules transition from a structured, closely packed liquid to a dispersed, high-velocity vapor. This transition results in a substantial increase in entropy, which can be thought of as the system's tendency toward increased disorder.

The change in entropy during vaporization (ΔS) is crucial for:

- Predicting spontaneity of phase changes.
- Calculating other thermodynamic properties.
- Understanding equilibrium conditions between phases.

Thermodynamic Relationship Between H and ΔS

The fundamental thermodynamic equation connecting enthalpy (H), entropy (S), and temperature (T) during phase transition is:

$$\Delta G = \Delta H - T \Delta S$$

At equilibrium during vaporization (boiling point), the Gibbs free energy change (ΔG) is zero:

$$0 = \Delta H_{\text{vap}} - T_{\text{vap}} \Delta S_{\text{vap}}$$

Rearranged, this yields:

$$\Delta S_{\text{vap}} = \frac{\Delta H_{\text{vap}}}{T_{\text{vap}}}$$

where:

- ΔH_{vap} is the heat of vaporization,
- T_{vap} is the temperature at which vaporization occurs (boiling point),
- ΔS_{vap} is the entropy change during vaporization.

This relationship provides a straightforward way to calculate the entropy change based on experimental data, assuming the vaporization occurs at a known temperature.

Calculating the Change in Entropy (ΔS) for Toluene Vaporization

Given Data and Assumptions

In this scenario, the heat of vaporization of toluene ($\text{C}_6\text{H}_5\text{CH}_3$) is:

$$\Delta H_{\text{vap}} = 38.1 \text{ kJ/mol}$$

To proceed with the calculation, we need the boiling point of toluene, which is approximately:

$$T_{\text{boiling}} = 110.6^\circ \text{C}$$

Converting to Kelvin:

$$T_{\text{boiling}} = 110.6 + 273.15 = 383.75 \text{ K}$$

Assumptions made:

- Vaporization occurs at the normal boiling point.
- The process is at equilibrium (standard conditions).
- The enthalpy of vaporization remains constant over the temperature range considered.

Step-by-Step Calculation

Using the thermodynamic relation:

$$\Delta S_{\text{vap}} = \frac{\Delta H_{\text{vap}}}{T_{\text{boiling}}}$$

Convert ΔH_{vap} into Joules per mole:

$$\Delta H_{\text{vap}} = 38.1 \text{ kJ/mol} = 38100 \text{ J/mol}$$

Plugging in the values:

$$\Delta S_{\text{vap}} = \frac{38100 \text{ J/mol}}{383.75 \text{ K}} \approx 99.2 \text{ J/(mol}\cdot\text{K)}$$

Result:

$$\boxed{\Delta S_{\text{vap}} \approx 99.2 \text{ J/(mol}\cdot\text{K)}}$$

This positive value indicates an increase in disorder as toluene transitions from liquid to vapor.

Implications and Further Considerations

Thermodynamic Significance of the Calculated ΔS

The entropy change of approximately 99.2 J/(mol·K) for toluene at its boiling point aligns with the expectation that vaporization involves increased molecular randomness. Such a substantial increase in entropy supports the spontaneity of vaporization at the boiling temperature, given that the process is endothermic (absorbs heat).

In practical terms, this entropy change also influences the vapor pressure of toluene and its behavior under varying temperature and pressure conditions. The Clausius-Clapeyron equation, which relates vapor pressure and temperature, depends on the heat of vaporization and the entropy change, highlighting their interconnectedness.

Limitations and Assumptions in the Calculation

While the calculation provides a good estimate, it is essential to recognize certain limitations:

- **Temperature Dependence of H:** The heat of vaporization decreases slightly with increasing temperature, so assuming a constant value over a broad temperature range introduces minor inaccuracies.
- **Ideal Behavior:** The calculation assumes ideal behavior, neglecting intermolecular deviations, vapor pressure variations, and non-idealities in real systems.
- **Pure Substance:** The calculation pertains to pure toluene at standard atmospheric pressure; mixtures or impurities can alter thermodynamic properties.

Relevance in Industrial and Environmental Contexts

Understanding the entropy change during vaporization has significant implications:

- Chemical Engineering: Design of distillation columns, solvent recovery, and phase separation processes relies on thermodynamic data.
- Environmental Science: Vaporization and volatilization influence pollutant dispersion, atmospheric reactions, and climate models.
- Material Science: Toluene's boiling and vaporization properties inform its use in manufacturing and material processing.

Conclusion: The Interplay of Heat, Entropy, and Molecular Dynamics

The calculation of the entropy change (ΔS) for toluene's vaporization exemplifies the elegant interplay between thermodynamic principles and molecular behavior. By leveraging the heat of vaporization and the boiling point, scientists and engineers can quantify the disorder introduced during phase transitions, informing both theoretical understanding and practical applications.

In this case, with a heat of vaporization of 38.1 kJ/mol and a boiling temperature of approximately 383.75 K, the entropy increases by roughly 99.2 J/(mol·K), reflecting a substantial rise in molecular disorder. This insight not only reinforces the fundamental concepts of thermodynamics but also underscores the importance of precise data and assumptions in predicting and controlling phase changes in chemical systems.

As industries continue to optimize processes and develop new materials, the foundational understanding of properties like H and ΔS remains indispensable, guiding innovations rooted in the laws of nature.

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