

Accepted Manuscript

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PII: S1004-9541(16)30020-9
DOI: doi: [10.1016/j.cjche.2016.05.004](https://doi.org/10.1016/j.cjche.2016.05.004)
Reference: CJCHE 557

To appear in:

Received date: 12 January 2016
Revised date: 3 May 2016
Accepted date: 9 May 2016

Please cite this article as: Chang-shuai Shen, Wen-li Li, Cai-rong Zhou, Investigation on molar heat capacity, standard molar enthalpy of combustion for guaiacol and acetyl guaiacol ester, (2016), doi: [10.1016/j.cjche.2016.05.004](https://doi.org/10.1016/j.cjche.2016.05.004)

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Investigation on molar heat capacity, standard molar enthalpy of combustion for guaiacol and acetyl guaiacol ester

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Abstract: The molar heat capacities (C_p) of guaiacol(CAS 90-50-1) and acetyl guaiacol ester (AGE, CAS 613-70-7) were determined from 290 K to 350 K by differential scanning calorimetry (DSC), and expressed as a function of temperature. Two kinds of group contribution models were used to estimate the molar heat capacities of both guaiacol and AGE, the average relative deviation is less than 10%. The standard molar enthalpies of combustion of guaiacol and AGE were $-3590.0 \text{ kJ}\cdot\text{mol}^{-1}$ and $-4522.1 \text{ kJ}\cdot\text{mol}^{-1}$ by a precise thermal isolation oxygen bomb calorimeter. The standard molar enthalpies of formation of guaiacol and AGE in a liquid state at 298.15 K were calculated to be $-307.95 \text{ kJ}\cdot\text{mol}^{-1}$ and $-448.72 \text{ kJ}\cdot\text{mol}^{-1}$, respectively, based on the standard molar enthalpies of combustion. The thermodynamic properties are useful for exploiting the new synthesis method, engineering design and industry production of AGE using guaiacol as a raw material.

Key words: Guaiacol; Acetyl guaiacol ester (AGE); Molar heat capacity; Standard molar enthalpy of combustion

List of symbols

- ε The heat capacity of calorimeter, $\text{J}\cdot\text{K}^{-1}$
- C The molar heat capacity of sample, $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$
- D The signal value of DSC for sample, mW
- H Enthalpy, $\text{kJ}\cdot\text{mol}^{-1}$
- m Mass of the tested sample, mg
- Q Quantity of heat, $\text{J}\cdot\text{mol}^{-1}$ or $\text{kJ}\cdot\text{mol}^{-1}$

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