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Atmospheric Chemistry and Physics Discussions

Interactive comment on "SIMPOL.1: A simple group contribution method for predicting vapor pressures and enthalpies of vaporization of multifunctional organic compounds" *by* J. F. Pankow and W. E. Asher

Anonymous Referee #3

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General comments

The manuscript presents a novel group contribution method for predicting saturation vapor pressures and vaporization enthalpies of organic compounds. The approach is based on fitting the values of the needed constants directly to available experimental data and as such it differs from the previous works of the authors where semi-empirical methods were used (Asher et al., 2002; Asher and Pankow, 2006). The study provides a simple and effective tool to estimate thermodynamic properties of various complex organics for which needed experimental data is lacking. This makes the

method also valuable for the atmospheric sciences community. Overall, I recommend the manuscript for publication in ACP after the authors have considered the following minor comments.

Specific comments

1. Introduction, page 11841, 3rd paragraph. The authors should mention the work of Tong et al. (“Thermodynamic Properties of Multifunctional Oxygenates in Atmospheric Aerosols from Quantum Mechanics and Molecular Dynamics: Dicarboxylic Acids”, Environ. Sci. Technol., 38, 3941-3949).

2. Section 3.4, pages 11854-11855. How does the performance of the fit depend on the temperature?

Technical corrections

1. Equation (6), page 11844. The value range of the parameter ‘k’ is mentioned twice.

2. Page 11851, line 19. The word “is” should be omitted.

Interactive comment on Atmos. Chem. Phys. Discuss., 7, 11839, 2007.