Supplementary information for the paper:

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Measurement and Prediction of Thermochemical Properties.

Improved Increments for the Estimation of Enthalpies of Sublimation and Standard Enthalpies of Formation of Alkyl Derivatives of Urea

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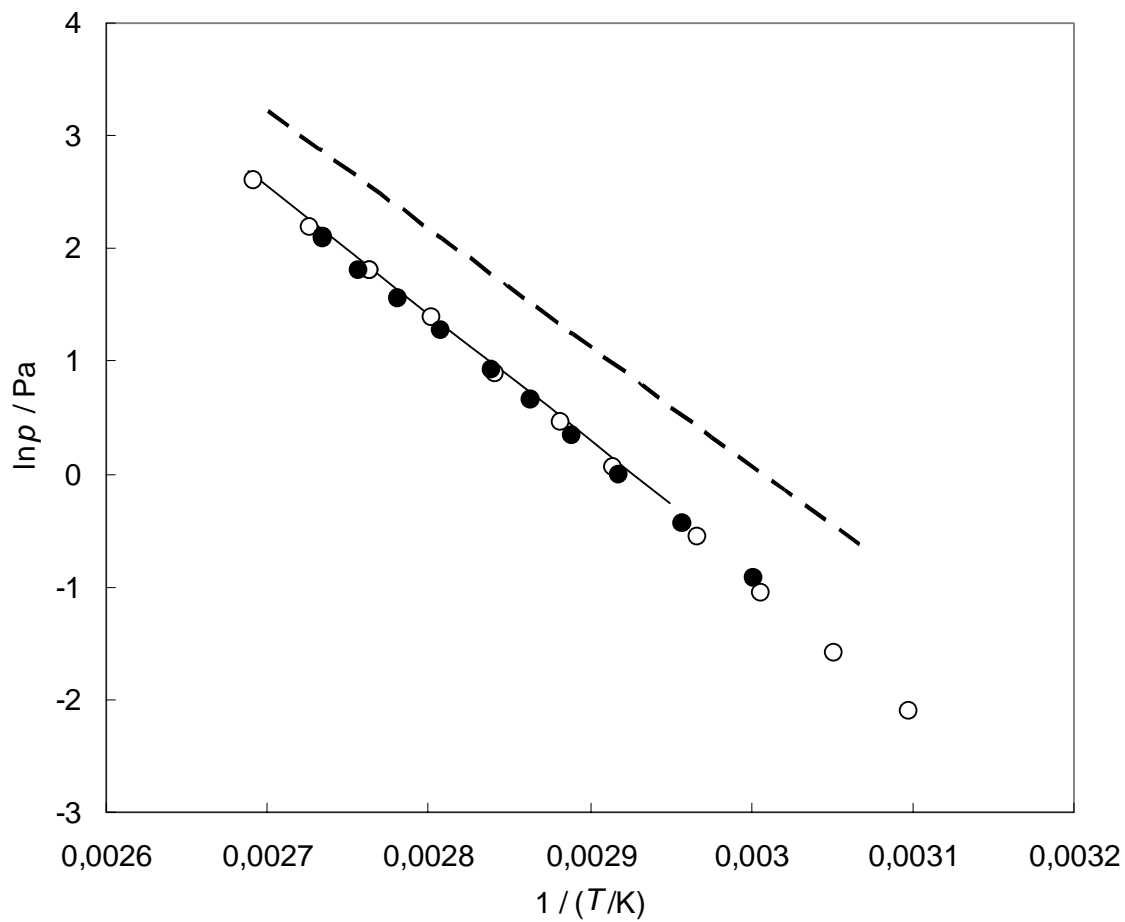[*]Corresponding author. E-mail: sergey.verevkin@uni-rostock.de

Figure 1. Experimental data of the vapor pressures of the 1-methylurea.

○   Zaitsau, 2003
●   this work
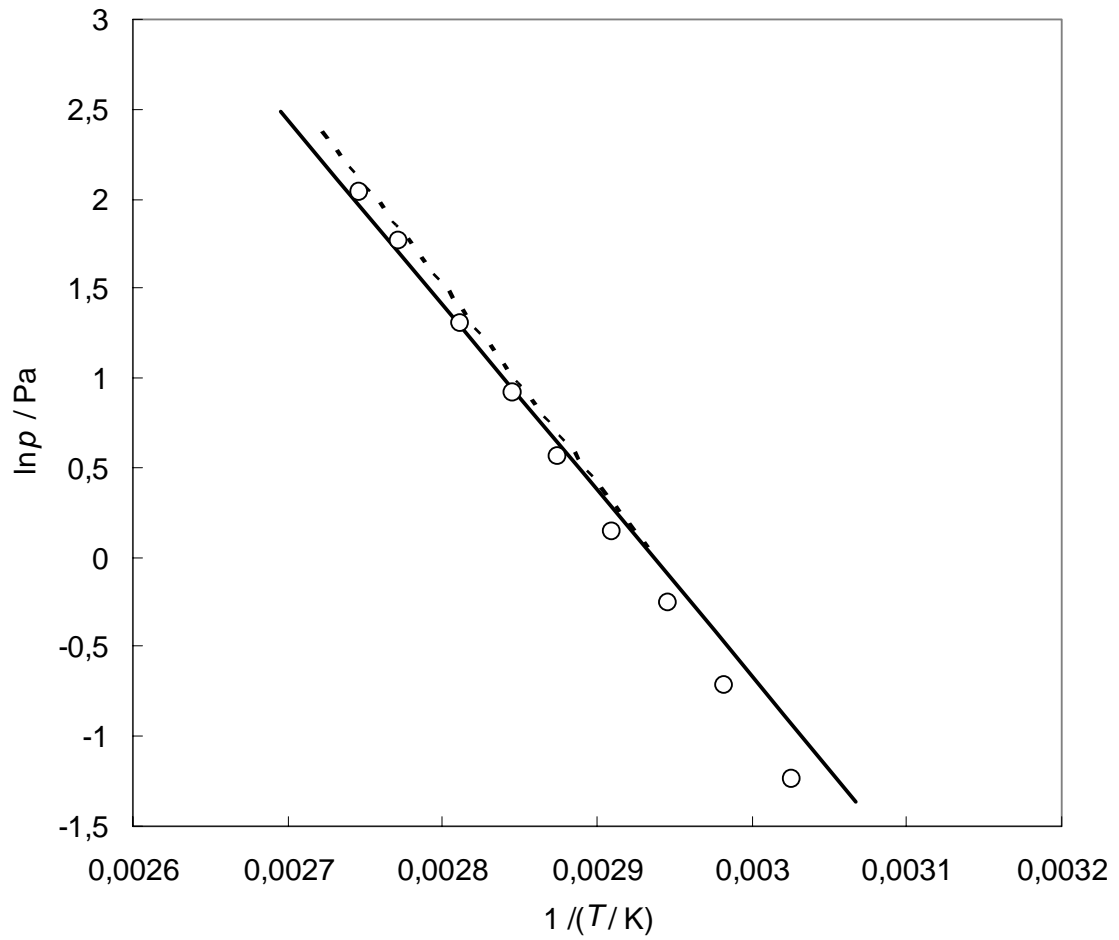----- Ferro, 1987
___   Piacente, 1990

Figure 2. Experimental data of the vapor pressures of the 1-ethylurea.

○   Zaitsau, 2003
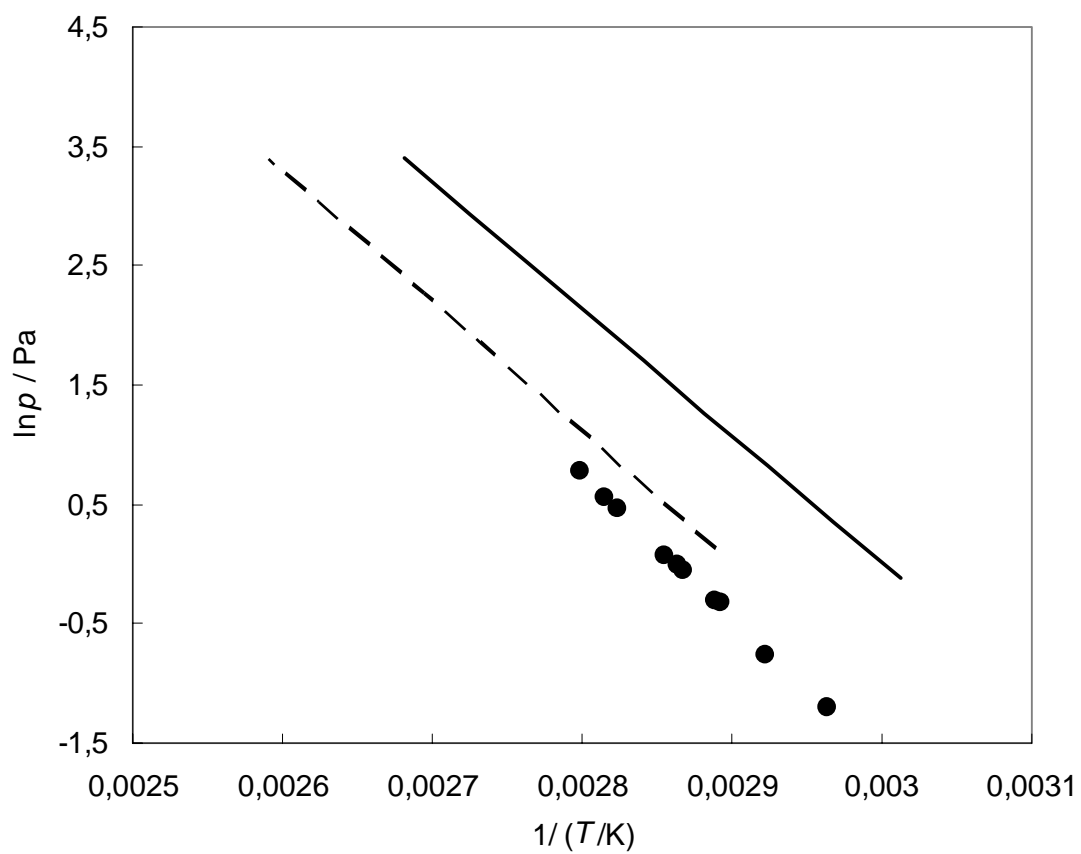-----   Piacente, 1990
___   Ferro, 1987

Figure 3. Experimental data of the vapor pressures of the 1-propylurea.

●   this work
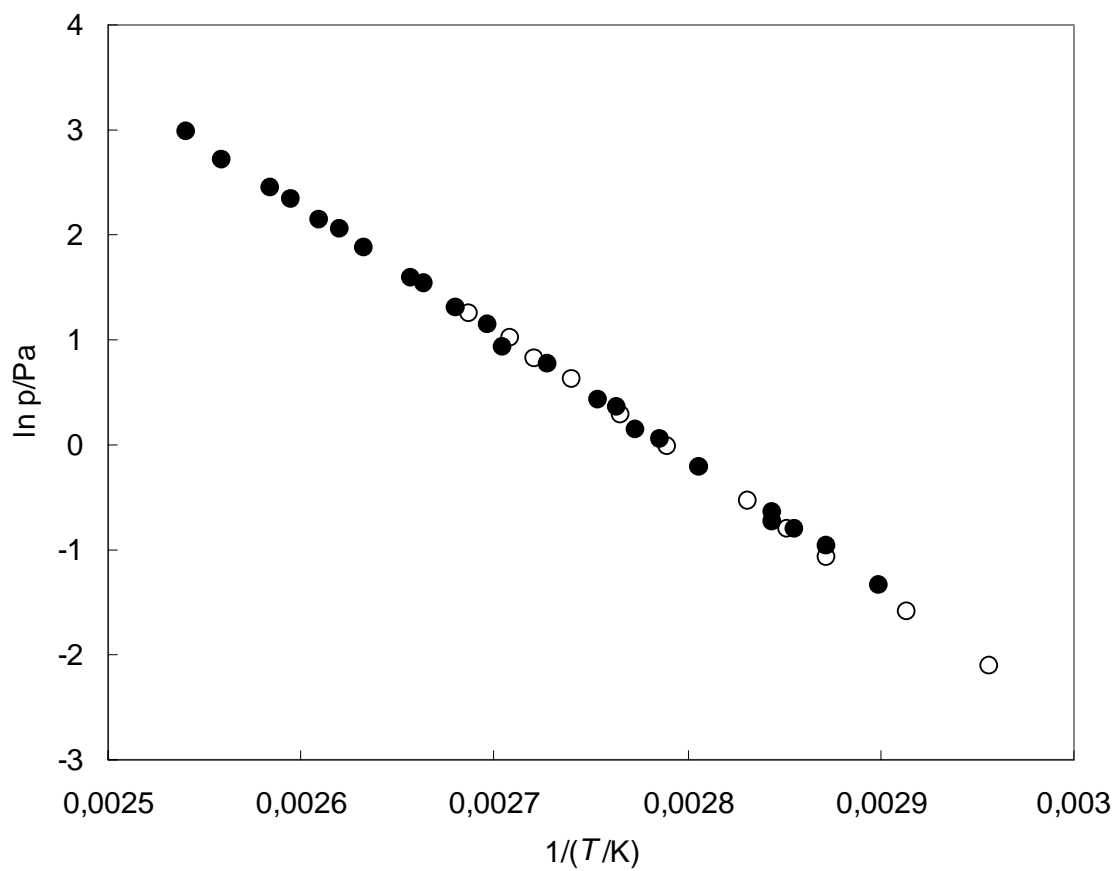-----   Piacente, 1990
___   Ferro, 1987

Figure 4. Experimental data of the vapor pressures of the sec-butylurea
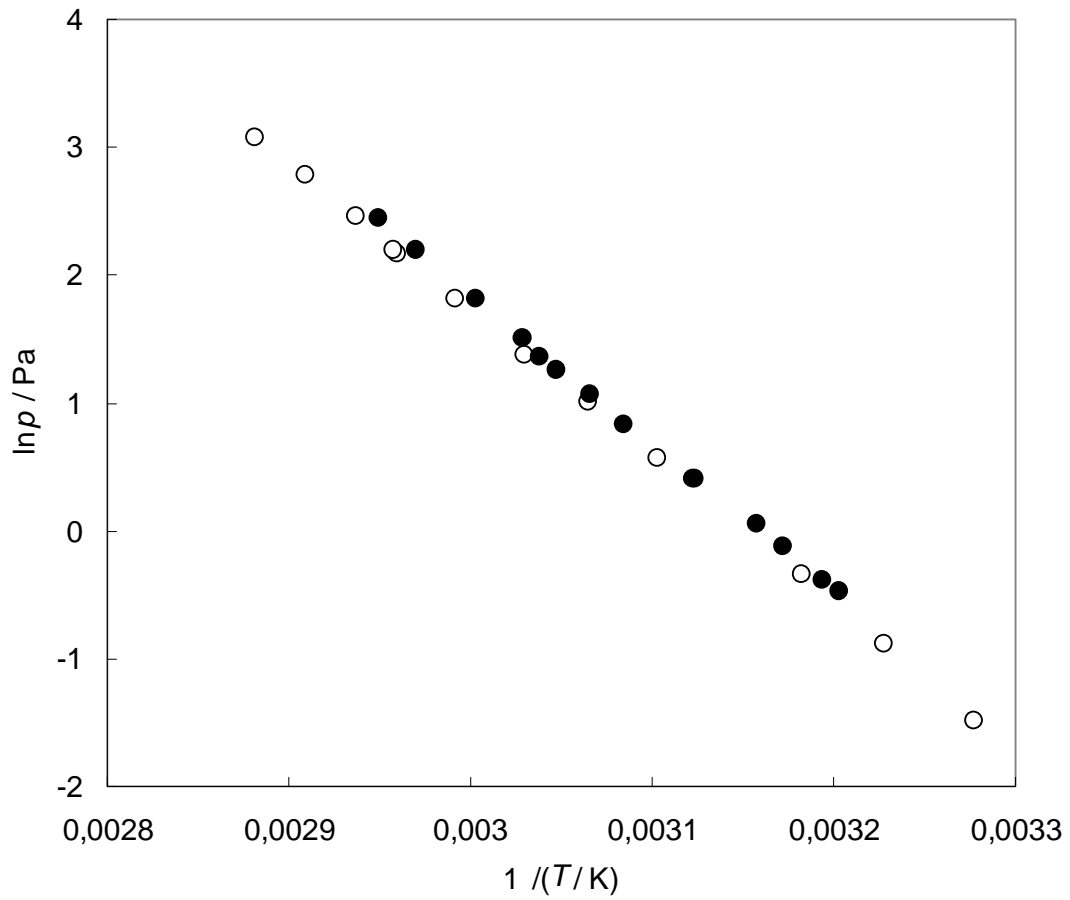
○   Zaitsau, 2003
●   this work

Figure 5. Experimental data of the vapor pressures of the 1,1-diethylurea

○   Zaitsau, 2003
●   this work

Figure 6. Experimental data of the vapor pressures of the 1,3-diethylurea.

○   Zaitsau, 2003
●   this work
-----   Ferro, 1987
___   Piacente, 1990

Figure 7. Experimental data of the vapor pressures of the 1,1-dimethylurea.

○   Zaitsau, 2003
●   this work
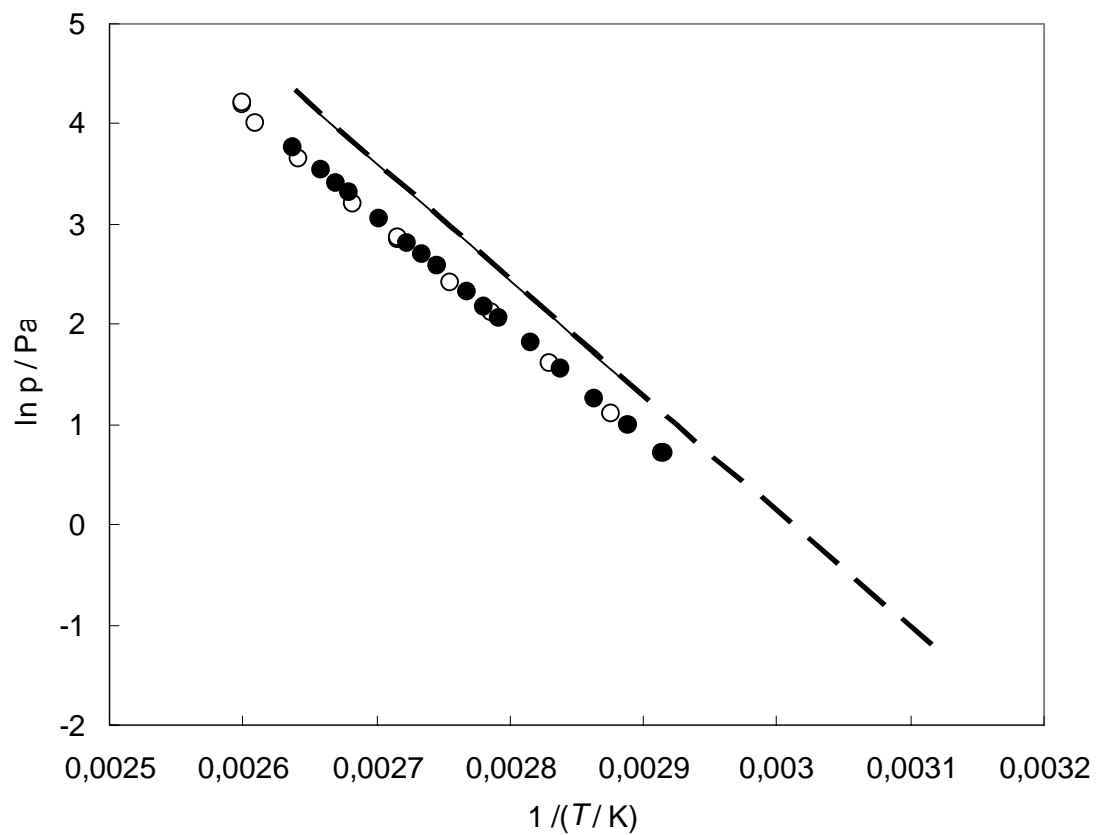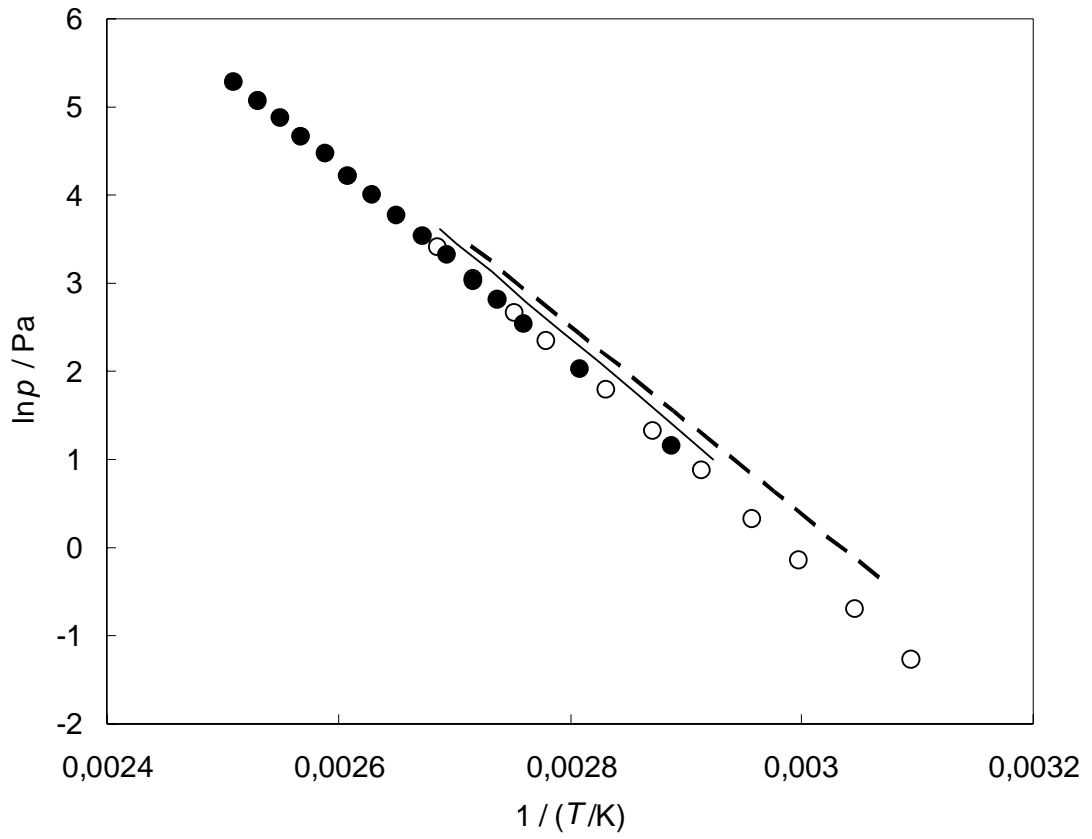-----   Ferro, 1987
___   Piacente, 1990

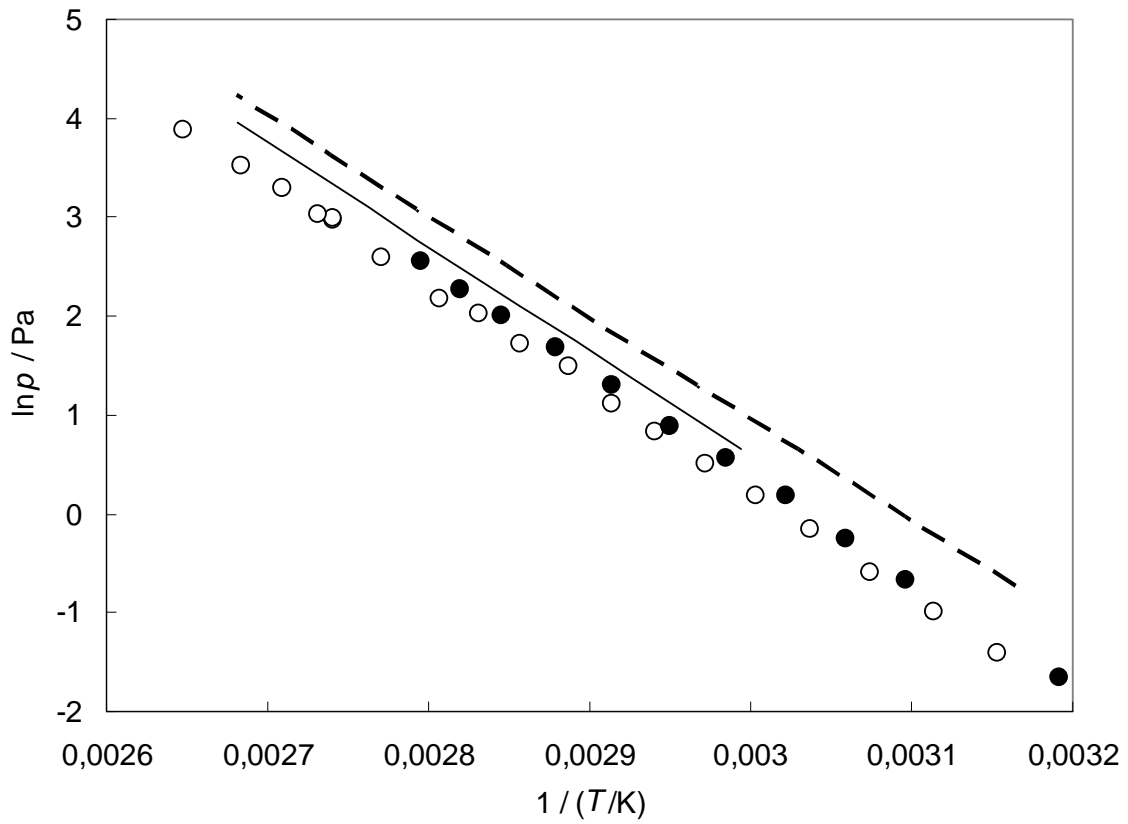Figure 8. Experimental data of the vapor pressures of the 1,3-dimethylurea

○   Zaitsau, 2003
●   this work
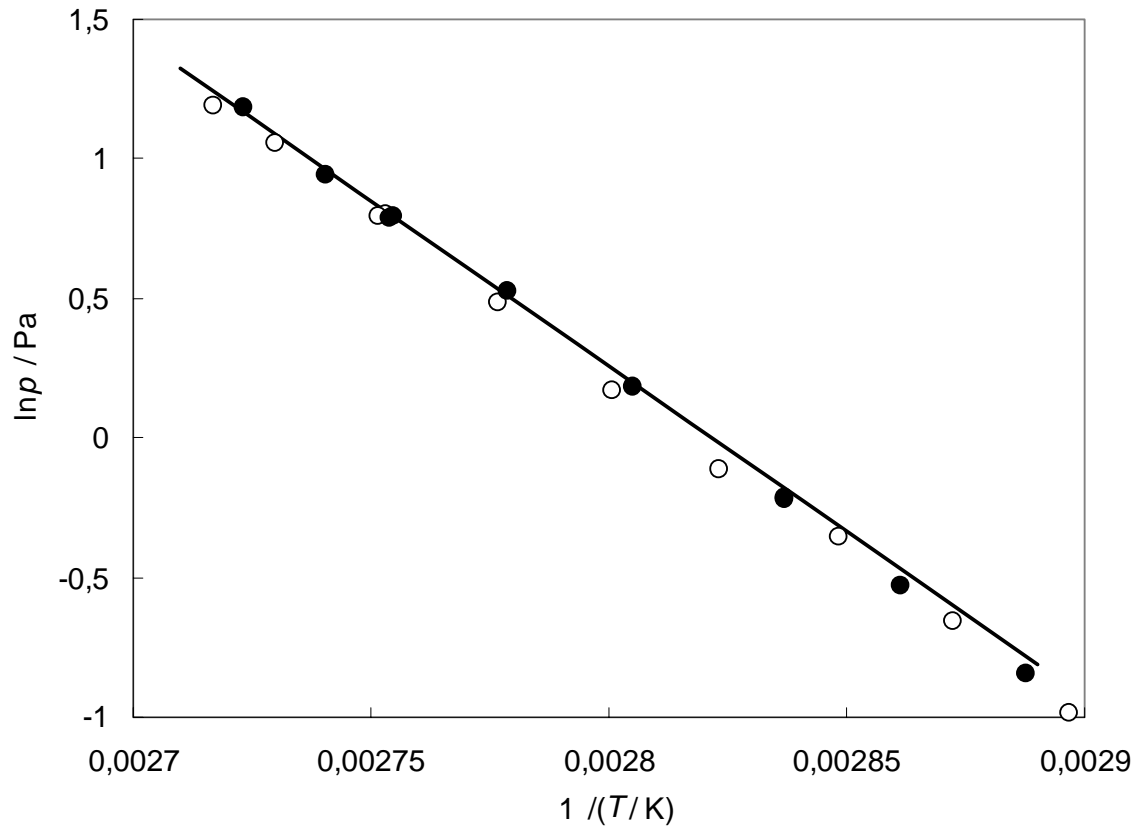----- Ferro, 1987
___   Piacente, 1990

Figure 9. Experimental data of the vapor pressures of the 1-butylurea.

○   Zaitsau, 2003.
●   this work
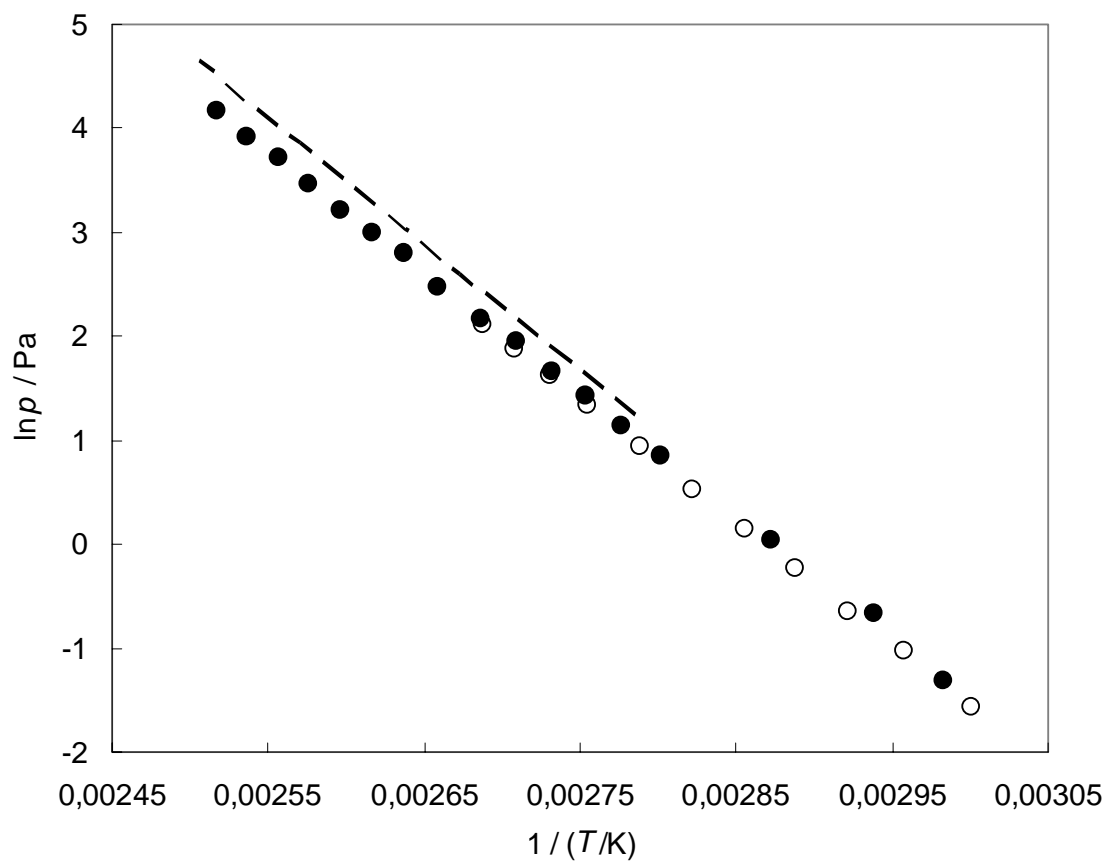___   Fiorani, 1987

Figure 10. Experimental data of the vapor pressures of the 1-tert-butylurea.

○   Zaitsau, 2003.
●   this work.
-----   Piacente, 1990

TABLE 1.

Group-contribution values calculated using $\Delta_f H_m^\circ$(cr)/ kJ mol^{-1} of urea and alkylureas (The experimental data and calculations from ref .5 (Simirskii, V. V.; Kabo, G. J.; Frenkel, M. L., Additivity of the enthalpies of formation of urea derivatives in the crystalline state. *J. Chem. Thermodyn.* **1987**, *19*, 1121-1127.)

Group-contribution	Set 1[a]	Set 2[b]
N-(H)$_2$(CO)	-466.45	-166.45
N-(H)(C)(CO)	-188.89	-91.22
N-(C)$_2$(CO)	-197.87	0.70
C-(H)$_3$(N)	22.62	-76.34
C-(H)$_2$(C)(N)	-19.75	-78.06
C-(H)(C)$_2$(N)	-62.89	-78.38
C-(C)$_3$(N)	-108.16	-81.92
C-(H)$_3$(C)	15.82	-25.48
C-(H)$_2$(C)$_2$	-29.38	-28.52

[a] The set of 10 entries: urea, 1-methylurea, 1-ethylurea, 1-iso-propylurea 1-n-butylurea, 1-sec-butylurea, 1-tert-butylurea, 1,1-di-methylurea, 1,1-di-ethylurea, and 1,3-di-tertbutylurea.
[b] The set of 9 entries: urea, 1-methylurea, 1-iso-propylurea 1-n-butylurea, 1-sec-butylurea, 1-tert-butylurea, 1,1-di-methylurea, 1,1-di-ethylurea, and 1,3-di-tertbutylurea (1-ethylurea is excluded).

TABLE 2. **Calculation of the Solid Enthalpy of Formation, $\Delta_f H_m^\circ$ (cr) for Alkyl Derivative of Urea at *T* = 298.15K (in kJ·mol^{-1}) using increments from ref. 31** (Domalski, E.S.; Hearing, E.D., Estimation of Thermodynamic Properties of C-H-N-O-Halogen Compounds at 298.15 K, *J. Phys. Chem. Ref. Data* **1993**, 22, 805-1159.)

Compounds	exp.	calc	exp-calc
1-methylurea	-327.80	-324.89	-2.91
1-ethylurea	-357.80	-358.89	1.09
1-iso-propylurea	-389.50	-390.21	0.71
1-n-butylurea	-419.50	-417.71	-1.79
1-sec-butylurea	-413.20	-417.28	4.08
1-tert-butylurea	-414.70	-430.42	15.72
1,1-dimethylurea	-319.10	-315.53	-3.57
1,1-diethylurea	-372.20	-374.83	2.63
		Mean:	4.06

TABLE 3. **Calculation of the Solid Enthalpy of Formation, $\Delta_f H_m^\circ$ (g) for Alkyl Derivative of Urea at T = 298.15K (in kJ·mol^{-1}) using increments from ref. 31** (Domalski, E.S.; Hearing, E.D., Estimation of Thermodynamic Properties of C-H-N-O-Halogen Compounds at 298.15 K, *J. Phys. Chem. Ref. Data* **1993**, 22, 805-1159.)

Compounds	exp.	calc	exp-calc
1-methylurea	-231.90	-232.54	0.64
1-ethylurea	-258.50	-260.84	2.34
1-iso-propylurea	-291.40	-296.02	4.62
1-n-butylurea	-314.50	-302.10	-12.40
1-sec-butylurea	-311.30	-314.39	3.09
1-tert-butylurea	-316.90	-330.45	13.55
1,1-dimethylurea	-224.20	-222.64	-1.56
1,1-diethylurea	-276.40	-270.12	-6.28
		Mean:	5.56