Journal of the Serbian Chemical Society
JSCS-info@shd.org.rs • www.shd.org.rs/JSCS
J. Serb. Chem. Soc. 75 (7) 997–1003 (2010)
JSCS–4025
UDC 547.21:536.423.1
Note

NOTE

Reliable prediction of heat of vaporization of *n*-alkanes at 298.15 K

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(Received 23 November 2009, revised 3 March 2010)

Abstract: A reliable model for the prediction of the heat of vaporization for *n*-alkanes at 298.15 K with the number of carbon atoms and normal boiling point as the only input parameters is recommended. The new model is compared with other literature models and was found to give the best results with absolute mean percentage deviation of 0.81 % and maximum absolute percentage deviation of 2.93 %.

Keywords: heat of vaporization; *n*-alkanes; prediction; model.

INTRODUCTION

The heat of vaporization, or enthalpy of vaporization, is the difference between the enthalpy of a saturated vapor and that of a saturated liquid at the same pressure and temperature. Heats of vaporization at the temperature T = 298.15 K, $\Delta H_{v,298}$, are essential parameters in thermodynamic studies. In many calculations associated with process design and simulation, it is necessary to known the physical and thermodynamic properties of pure compounds, including their heat of vaporization. The accurate prediction of the heat of vaporization $\Delta H_{v,298}$ for hydrocarbon fluids is of particular interest in the petroleum industry.

The objective of this work was to develop a reliable predictive model for the estimation of the heat of vaporization $\Delta H_{v,298}$ of *n*-alkanes.

EXISTING MODELS

Many prediction models for the heat of vaporization have been proposed in the past. The majority of these models are applicable only at T = 298.15 K, or to a specific group of compounds. Most of the later ones are applicable only to *n*-alkanes. In these models, the critical temperature, T_c, critical pressure, p_c, triple point temperature, T_t, normal boiling point, T_b, and heat of vaporization at the

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doi: 10.2298/JSC091123067J

normal boiling point, ΔH_{vb}, as well as molar weight, M, and number of carbon atoms, n_c, are the input parameters.

NEW MODEL

Experimental values for many of the above-mentioned input parameters for higher *n*-alkanes are non-existent. However, experimental normal boiling point, T_b, is usually a known and a reliable parameter.

The experimental calorimetric heat of vaporization data for *n*-alkanes at 298.15 K and the experimental normal boiling points used are listed in Table I.

TABLE I. Experimental data

Compound	n_c	T_b / K	$\Delta H_{v,exp}$ / J mol^{-1}	Ref.
Pentane	5	309.2	26423.1	1
			26427.0	2
			26217.7	3
			26870.0	4
			26628.0	5
Hexane	6	341.9	31550.0	6
			31568.5	7
			30993.6	8
			31545.5	1
Heptane	7	371.6	36580.0	6
			36542.4	1
			36547.0	9
			36610.0	4
Octane	8	398.8	41470.0	6
			41528.9	10
			41478.8	1
			41616.8	11
			40988.8	12
			41491.2	13
			41449.3	13
			41491.2	14
			41340.0	15
			41491.2	16
Nonane	9	424.0	46431.6	1
			46420.0	4
Decane	10	447.3	51380.4	10
			51358.8	1
			50241.6	12
			50116.0	12
			51288.3	13
			51037.1	13
			50702.1	13
			50576.5	13
			50450.9	13
			51380.0	17

TABLE I. Continued

Compound	n_c	T_b / K	$\Delta H_{v,exp}$ / J mol^{-1}	Ref.
Decane			51390.0	18
			51360.0	19
Undecane	11	469.1	56471.6	10
			56312.5	13
			56019.4	13
			55935.6	13
			55475.1	13
			55768.2	13
			55517.0	13
			56440.0	17
			56770.0	20
Dodecane	12	489.1	61780.0	21
			61336.6	22
			59536.3	12
			60876.1	13
			60499.3	13
			60457.4	13
			60331.8	13
			61270.0	18
Tridecane	13	508.6	66402.6	22
Tetradecane	14	526.7	71133.7	22
			68998.5	12
			68789.9	12
			68705.4	12
			70463.8	13
			70338.2	13
			69668.3	13
			69584.6	13
			71008.1	23
Pentadecane	15	543.8	76241.6	22
			76800.0	24
Hexadecane	16	560.0	81433.3	22
			81400.0	24
			67993.6[a]	12
			70673.2[a]	12
			79716.7	13
			78711.8	13
			79591.1	13
			78586.2	13
			80700.0	25
			80600.0	20
Heptadecane	17	575.2	86080.6	22
			86500.0	24
Octadecane	18	589.9	91400.0	24
Nonadecane	19	603.0	96400.0	24
Eicosane	20	617.0	101800.0	24

TABLE I. Continued

Compound	n_c	T_b / K	$\Delta H_{v,exp}$ / J mol^{-1}	Ref.
Heneicosane	21	629.7	109400.0[a]	24
			106800.0	26
Docosane	22	641.8	115600.0[a]	24
			111900.0	26
Tricosane	23	653.2	120500.0[a]	24
			117000.0	26
Tetracosane	24	664.5	125600.0[a]	24
			121900.0	26
Pentacosane	25	675.1	126900.0	24
			126800.0	26
Hexacosane	26	685.0	139100.0[a]	24
			131700.0	26
Heptacosane	27	695.4	145100.0[a]	24
			135600.0	26
Octacosane	28	704.8	151400.0[a]	24
			141900.0	26
Nonacosane	29	714.0	147100.0	26
Triacontane	30	722.9	162900.0[a]	24
			152300.0	26
Hentriacontane	31	732.2[b]	157300.0	27
Dotriacontane	32	740.2	162500.0	27
Tritriacontane	33	748.5[b]	167600.0	27
Tetratriacontane	34	756.0	172700.0	27
Pentatriacontane	35	763.2	178100.0	27
Hexatriacontane	36	771.0	182900.0	27
Heptatriacontane	37	778.0	187600.0	27
Octatriacontane	38	785.0	192700.0	27

[a]Not used in the correlation; [b]estimated by the Kreglewski–Gamba–Soave–Pellegrini method[28]

Data from Table I were used for the development of a reliable predictive model for the estimation of the heat of vaporization, $\Delta H_{v,298}$, of *n*-alkanes:

$$\Delta H_{v,298}[\text{J/mol}] = 5684.27 + 5295.41 n_c - 17.2732 T_b \quad (1)$$

RESULTS AND DISCUSSION

The estimation capability of the new model was compared with that of other models and the results are presented in Table II. The absolute mean percent deviation is defined as:

$$p_{av} = (100 / N) \sum_{i=1}^{N} \left| (\Delta H_{v,298,exp} - \Delta H_{v,298,cal}) / \Delta H_{v,298,exp} \right| \quad (2)$$

The maximum absolute percent deviations are listed in the last column of Table II. The results presented in Table II indicate that the new model is the best predictive model for heat of vaporization of *n*-alkanes at 298.15 K.

Table II. Comparison of the Models

Model	Input parameters	p_{av} / %	p_{max} / %
Dunkel[29]	*GC*[a]	7.66	14.83
Laidler-Lovering-Nor-McCurdy[30-33]	*GC*	1.25	3.09
Klages[34]	T_b	14.47	48.23
Klages-Wadsö[35]	T_b	10.99	43.54
Abramzon[36]	*GC*	2.57	6.91
Wall-Flynn-Straus[37]	n_c	7.43	27.38
Morawetz[22]	n_c	0.87	3.78
Månsson-Sellers-Stridh-Sunner[38]	n_c	0.92	3.68
Ducros-Gruson-Sannier[39-42]	*GC*	0.95	3.47
Chickos-Hyman-Ladon-Liebman I[43]	n_c	3.83	7.03
Chickos-Hyman-Ladon-Liebman II[43]	*n*c	2.89	6.67
Guthrie-Taylor I[44]	*GC*	1.06	3.17
Guthrie-Taylor II[44]	*GC*	1.51	5.06
Constantinou-Gani[45]	*GC*	3.19	10.65
Chickos-Wilson[24]	n_c	3.55	10.43
Marano-Holder[46]	n_c	0.92	3.57
Phillips[47]	*M*	10.58	26.46
Marrero-Gani[48]	*GC*	1.12	3.47
Chickos-Hanshaw[27]	n_c	0.92	4.22
Kolská-Růžička-Gani[49]	*GC*	2.56	8.23
This model	n_c, *T*b	0.81	2.93

[a]Group contributions

CONCLUSIONS

The experimental values of the heat of vaporization of *n*-alkanes at 298.15 K, together with appropriate literature predictive models are reviewed in this work. A new reliable predictive model with two input parameters was developed. The obtained results indicate that the model with only two input parameters, one structural (n_c) and one property (T_b) parameter, gave a more reliable prediction of the heat of vaporization than the model with only one input parameter.

Acknowledgement. The authors gratefully acknowledge the financial support received from the Research Fund of the Ministry of Science and Technological Development of the Republic of Serbia and the Faculty of Technology and Metallurgy, University of Belgrade (project No 142064).

NOMENCLATURE

n_c Number of carbon atom
M Molar weight, g mol^{-1}
T_t Triple point temperature, K
T_c Critical temperature, K
p_c Critical pressure, bar
ω Acentric factor
ΔH_{vb} Heat of vaporization at normal boiling point, J mol^{-1}
$\Delta H_{v,298}$ Heat of vaporization at 298.15 K, J mol^{-1}

N Number of data points
p_{av} Absolute mean percent deviation, %
p_{max} Maximum absolute percent deviation, %

ИЗВОД

ПОУЗДАН МОДЕЛ ЗА ПРЕДСКАЗИВАЊЕ ТОПЛОТЕ ИСПАРАВАЊА *n*-АЛКАНА НА 298,15 K

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У овом раду предложен је поуздан модел за процену вредности топлоте испаравања *n*-алкана на температури 298,15 K са бројем угљеникових атома и нормалном температуром кључања, као јединим потребним вредностима. Предложени модел упоређен је са постојећим одговарајућим моделима и дао је најбоље, како средње процентуално одступање 0,81 %, тако и најмању вредност максималног процентуалног одступања 2,93 %.

(Примљено 23. новембра 2009, ревидирано 3. марта 2010)

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