Molecular Electronegative Distance Vector (MEDV) Related to 15 Properties of Alkanes

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Several quantitative structure−property relationship (QSPR) models between 15 basic physical properties or thermodynamic functions of alkanes and their molecular electronegative distance vectors (MEDV) are developed. For six of the properties—boiling point (BP), density (*D*) at 25 °C, refraction index (RI) at 25 °C, critical temperature (CT), critical pressure (CP), and surface tension (ST) at 20 °C—logarithmic models are found to give better results than conventional (linear) models since the values of these properties all tend to a limit with increasing carbon chain length. All models are created using multiple linear regression (MLR). Conventional models are proposed for the remaining nine physical properties or thermodynamic functions: molar volume (MV) at 20 °C, molar refraction (MR) at 20 °C, heat capacity (HC) at 300 K, enthalpy (*E*) at 300 K, heats of vaporization (HV) at 25 °C, heat of atomization (HA) at 25 °C, standard heat of formation (HF) at 25 °C, heat of formation in liquid (HFL) at 25 °C, and heat of formation in gas (HFG) at 25 °C.

INTRODUCTION

Determination of physicochemical properties including thermodynamic functions for chemical and chemical engineering substances plays an important role in finding or building structure−property relationships of many compounds, mainly organic compounds, and has become a major interest of many chemists and scientists in recent years.[1−4] A vast amount of physical properties for a number of compounds have been obtained in many laboratories, and several standard databases such as DIPPR[5,6] have been built. However, it is still difficult to determine accurately the physical properties of some substances which are unstable thermodynamically or difficult to synthesize or purify. As a result, many methods using quantitative structure−property relationships (QSPRs) have been proposed to estimate the physicochemical properties of these compounds in recent years.[7−11] Despite the amount of literature available on the subject of QSPRs,[12−14] many existing structural parametrization schemes need further improvement. One of the most important structural parametrization methods is the use of topological indices based on molecular graphs of organic compounds. More than 100 topological indices including Hosoya index, Randic indices, Wiener index, etc. have been developed and have been applied widely in QSPR studies.[15−22] To obtain excellent QSPR models, it is often necessary to choose descriptors from a pool composed of many structural descriptors using various optimization methods including neural network,[23,24] simulation annealing,[25] genetic algorithm,[26] and so on. For example, Wessel and Jurs[27] selected six structural descriptors from a pool composed of 81 variables by using a Gram−Schmidt orthogonalization method and a genetic algorithm feature selection routine to create a six-variable model that linked normal boiling points of alkanes. However, this is tedious and time-consuming. In addition, many of the indices come from the topological distance matrix and the geometric distance matrix is often described as a number for the examined compounds and so decreases the discrimination information for varied isomers. Therefore, the λ vector containing 10 elements used to describe the structure of alkanes was proposed in our previous paper, and this λ vector was related to boiling point,[28] six physical properties,[29] gas chromatographic indices,[30] and thermodynamic functions of alkanes[31] with good results. Afterward, the vector was modified and extended to systems containing heteroatoms such as oxygen.[32]

In this paper, a novel molecular electronegative distance vector, the MEDV proposed in our previous paper,[33] will be utilized to develop several QSPR models for 150 alkanes using multiple linear regression (MLR). It has been found that the MEDV has a good discrimination with no identical one for 150 alkane isomers containing carbon atom numbers from 1 through 10, and there is also a high correlation between the MEDV and many physical properties and thermodynamic functions such as boiling point (BP), density (*D*) at 25 °C, refraction index (RI) at 25 °C, critical temperature (CT), critical pressure (CP), surface tension (ST) at 20 °C, molar volume (MV) at 20 °C, molar refraction (MR) at 20 °C, heat capacity (HC) at 300 K, enthalpy (*E*) at 300 K, heats of vaporization (HV) at 25 °C, heat of atomization (HA) at 25 °C, standard heat of formation (HF) at 25 °C, heat of formation in liquid (HFL) at 25 °C, and heat of formation in gas (HFG) at 25 °C.

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Table 1. All Relative Distances of 2,2,3-Trimethylpentane Used in Eq 1

no.	*k*	*l*	*d*(*i*,*j*)									
1	1	1	2(1,6)	2(1,7)	3(1,8)	4(1,5)	2(6,7)	3(6,8)	4(6,5)	3(7,8)	4(7,5)	3(8,5)
2	1	2	3(1,4)	3(6,4)	3(7,4)	2(8,4)	1(5,4)					
3	1	3	2(1,3)	2(6,3)	2(7,3)	1(8,3)	2(5,3)					
4	1	4	1(1,2)	1(6,2)	1(7,2)	2(8,2)	3(5,2)					
5	2	2	no									
6	2	3	1(4,3)									
7	2	4	2(4,2)									
8	3	3	no									
9	3	4	1(3,2)									
10	4	4	no									

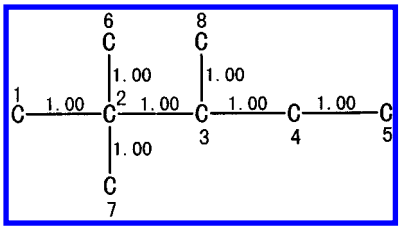

Figure 1. Description of skeletal structure of the 2,2,3-trimethylpentane molecule.

THEORETICAL SECTION

The MEDV of Alkanes. According to the literature,[33] to construct a MEDV of an organic molecule, it is essential to specify various *atomic types* and *atomic attributes* of all non-hydrogen atoms in the examined molecule. If an atom is linked to *k* ($k = 1, 2, 3, 4$) non-hydrogen atom/atoms through chemical bond/bonds, then *atomic type* of the atom belongs to *k*. The term "atomic attribute" of an atom is used to represent the chemical element type and chemical bond type of the atom. For the alkanes examined in our present paper, there are four atomic types and only one atomic attribute, i.e., a sp^3 carbon atom. Therefore, the *relative electronegativities* of all non-hydrogen atoms are $q = 1.0000$ and the *relative bond length* between two adjacent non-hydrogen atoms is $d = 1.0000$ (see Figure 1). Thus the eight non-hydrogen atoms in the molecule 2,2,3-trimethylpentane belong to atomic type 1, 4, 3, 2, 1, 1, 1, and 1, respectively. Therefore, the formula of the MEDV for alkanes can be simplified as:

$$m_{kl} = \sum_{i\in k,\, j\in l} \frac{q_i q_j}{d_{ij}^2} = \sum_{i\in k,\, j\in l} \frac{1}{d_{ij}^2} \quad (k = 1, 2, 3, 4;\ l \geq k;\ k \leq 4) \tag{1}$$

where *k* or *l* is an atomic type of an atom, and *i* or *j* is a coding number or series number of an atom in the molecular skeleton graph; *i* belongs to the *k*th atomic type and *j* belongs to the *l*th atomic type. d_{ij} refers to the relative distance of the shortest path between the *i*th atom and the *j*th atom. All d_{ij} values for the sample molecule 2,2,3-trimethylpentane are shown in Table 1. From the definition in eq 1, there are 10 elements, m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34} and m_{44}, in the MEDV for all alkane molecules. The 10 elements are noted x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9, x_{10}, respectively. From Table 1 and eq 1, the 10 elements are obtained as follows.

$$x_2 = m_{12} = \frac{1}{3^2} + \frac{1}{3^2} + \frac{1}{3^2} + \frac{1}{2^2} + \frac{1}{1^2} = 1.5833$$

$$x_1 = m_{11} = \frac{1}{2^2} + \frac{1}{2^2} + \frac{1}{3^2} + \frac{1}{4^2} + \frac{1}{2^2} + \frac{1}{3^2} + \frac{1}{4^2} + \frac{1}{3^2} + \frac{1}{4^2} + \frac{1}{3^2} = 1.3819$$

$$x_3 = m_{13} = \frac{1}{2^2} + \frac{1}{2^2} + \frac{1}{2^2} + \frac{1}{1^2} + \frac{1}{2^2} = 2.0000$$

$$x_4 = m_{14} = \frac{1}{1^2} + \frac{1}{1^2} + \frac{1}{1^2} + \frac{1}{2^2} + \frac{1}{3^2} = 3.3611$$

$$x_5 = m_{22} = 0, \quad x_6 = m_{23} = \frac{1}{1^2} = 1.0000$$

$$x_7 = m_{24} = \frac{1}{2^2} = 0.2500, \quad x_8 = m_{33} = 0$$

$$x_9 = m_{34} = \frac{1}{1^2} = 1.000, \quad x_{10} = m_{44} = 0$$

QSPR Models. It has been found that a number of physical properties or thermodynamic functions of a compound depend on its structure. The above MEDV containing 10 elements is also a kind of structural descriptor and can be used to create a QSPR model. The relationship between the structural descriptor (MEDV), x_i, and property (y), physical property or thermodynamic function, can be written as eq 2A or eq 2B:

$$y = b_0 + \sum_{i=1}^{10} b_i x_i \tag{2A}$$

$$\ln(\text{opt} - y) = b_0 + \sum_{i=1}^{10} b_i x_i \tag{2B}$$

where b_i ($i = 0, 1, 2, ..., 10$) are regression coefficients and "opt" is a limited value of a kind of property. The b_i values are calculated using multiple linear regression (MLR). Various statistics such as correlation coefficient (R) and root-mean-square error (rms) are also estimated simultaneously by eqs 3A and 3B:

$$R = \sqrt{1 - \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 / \sum_{i=1}^{n} (y_i - \bar{y})^2} \tag{3A}$$

$$\text{rms} = \sqrt{\sum_{i=1}^{n} (\hat{y}_i - y_i)^2 / n} \tag{3B}$$

Table 2. 150 Alkanes and Their MEDV Values

no.	compound	m_{11}	m_{12}	m_{13}	m_{14}	m_{22}	m_{23}	m_{24}	m_{33}	m_{34}	m_{44}
1	methane	0	0	0	0	0	0	0	0	0	0
2	ethane	1.0000	0	0	0	0	0	0	0	0	0
3	propane	0.2500	2.0000	0	0	0	0	0	0	0	0
4	butane	0.1111	2.5000	0	0	1.0000	0	0	0	0	0
5	2-methylpropane	0.7500	0	3.0000	0	0	0	0	0	0	0
6	pentane	0.0625	2.7222	0	0	2.2500	0	0	0	0	0
7	2-methylbutane	0.4722	1.5000	2.2500	0	0	1.0000	0	0	0	0
8	2,2-dimethylpropane	1.5000	0	0	4.0000	0	0	0	0	0	0
9	hexane	0.0400	2.8472	0	0	3.6111	0	0	0	0	0
10	2-methylpentane	0.3750	1.9722	2.1111	0	1.0000	1.2500	0	0	0	0
11	3-methylpentane	0.2847	2.7222	1.5000	0	0.2500	2.0000	0	0	0	0
12	2,2-dimethylbutane	1.0833	1.7500	0	3.2500	0	0	1.0000	0	0	0
13	2,3-dimethylbutane	0.9444	0	5.0000	0	0	0	0	1.0000	0	0
14	heptane	0.0278	2.9272	0	0	5.0347	0	0	0	0	0
15	2-methylhexane	0.3300	2.2083	2.0625	0	2.2500	1.3611	0	0	0	0
16	3-methylhexane	0.2136	3.0972	1.3611	0	1.3611	2.2500	0	0	0	0
17	2,2-dimethylpentane	0.9375	2.3333	0	3.1111	1.0000	0	1.2500	0	0	0
18	2,3-dimethylpentane	0.7083	1.4722	4.1111	0	0	1.2500	0	1.0000	0	0
19	2,4-dimethylpentane	0.7500	1.0000	4.4444	0	0	2.0000	0	0.2500	0	0
20	3,3-dimethylpentane	0.7569	3.2222	0	2.5000	0.2500	0	2.0000	0	0	0
21	3-ethylpentane	0.1875	3.6667	0.7500	0	0.7500	3.0000	0	0	0	0
22	2,2,3-trimethylbutane	1.6667	0	2.7500	3.5000	0	0	0	0	1.0000	0
23	octane	0.0204	2.9828	0	0	6.4983	0	0	0	0	0
24	2-methylheptane	0.3056	2.3508	2.0400	0	3.6111	1.4236	0	0	0	0
25	3-methylheptane	0.1789	3.2883	1.3125	0	2.6736	2.3611	0	0	0	0
26	4-methylheptane	0.1528	3.4272	1.2222	0	2.5347	2.5000	0	0	0	0
27	2,2-dimethylhexane	0.8700	2.6319	0	3.0625	2.2500	0	1.3611	0	0	0
28	2,3-dimethylhexane	0.6147	1.9583	3.9236	0	1.0000	1.6111	0	1.0000	0	0
29	2,4-dimethylhexane	0.5661	2.2361	3.6458	0	0.2500	3.1111	0	0.2500	0	0
30	2,5-dimethylhexane	0.6600	1.4444	4.2500	0	1.0000	2.5000	0	0.1111	0	0
31	3,3-dimethylhexane	0.6372	3.7083	0	2.3611	1.3611	0	2.2500	0	0	0
32	3,4-dimethylhexane	0.4983	2.8472	3.2222	0	0.1111	2.5000	0	1.0000	0	0
33	3-ethylhexane	0.1425	3.9444	0.6111	0	1.9722	3.2500	0	0	0	0
34	2,2,3-trimethylpentane	1.3819	1.5833	2.0000	3.3611	0	1.0000	0.2500	0	1.0000	0
35	2,2,4-trimethylpentane	1.3750	1.2500	2.3333	3.2222	0	1.0000	1.0000	0	0.2500	0
36	2,3,3-trimethylpentane	1.2917	1.7222	2.6111	2.7500	0	0.2500	1.0000	0	1.0000	0
37	2,3,4-trimethylpentane	1.1944	0	6.9444	0	0	0	0	2.2500	0	0
38	2-methyl-3-ethylpentane	0.5625	2.6667	3.2222	0	0.2500	2.5000	0	1.0000	0	0
39	3-methyl-3-ethylpentane	0.5208	4.4167	0	1.7500	0.7500	0	3.0000	0	0	0
40	2,2,3,3-tetramethylbutane	2.5000	0	0	7.5000	0	0	0	0	0	1.0000
41	nonane	0.0156	3.0236	0	0	7.9897	0	0	0	0	0
42	2-methyloctane	0.2908	2.4464	2.0278	0	5.0347	1.4636	0	0	0	0
43	3-methyloctane	0.1593	3.4064	1.2900	0	4.0747	2.4236	0	0	0	0
44	4-methyloctane	0.1229	3.5939	1.1736	0	3.8872	2.6111	0	0	0	0
45	2,2-dimethylheptane	0.8333	2.8144	0	3.0400	3.6111	0	1.4236	0	0	0
46	2,3-dimethylheptane	0.5678	2.2119	3.8525	0	2.2500	1.7847	0	1.0000	0	0
47	2,4-dimethylheptane	0.4931	2.6286	3.4844	0	1.3611	3.4236	0	0.2500	0	0
48	2,5-dimethylheptane	0.4967	2.5869	3.4775	0	1.3611	3.5625	0	0.1111	0	0
49	2,6-dimethylheptane	0.6111	1.6944	4.1600	0	2.2500	2.7222	0	0.0625	0	0
50	3,3-dimethylheptane	0.5800	3.9619	0	2.3125	2.6736	0	2.3611	0	0	0
51	3,4-dimethylheptane	0.4150	3.2883	3.0347	0	1.1736	2.8611	0	1.0000	0	0
52	3,5-dimethylheptane	0.3925	3.4272	2.8472	0	0.5625	4.2222	0	0.2500	0	0
53	4,4-dimethylheptane	0.5278	4.1494	0	2.2222	2.5347	0	2.5000	0	0	0
54	3-ethylheptane	0.1181	4.0906	0.5625	0	3.3472	3.3611	0	0	0	0
55	4-ethylheptane	0.1078	4.1772	0.4722	0	3.2569	3.5000	0	0	0	0
56	2,2,3-trimethylhexane	1.2658	2.1319	1.8611	3.3125	1.0000	1.2500	0.3611	0	1.0000	0
57	2,2,4-trimethylhexane	1.1686	2.5486	1.5833	3.1736	0.2500	2.0000	1.1111	0	0.2500	0
58	2,2,5-trimethylhexane	1.2400	1.8056	2.1875	3.1250	1.0000	1.2500	1.2500	0	0.1111	0
59	2,3,3-trimethylhexane	1.1494	2.3194	2.5625	2.6111	1.0000	0.3611	1.2500	0	1.0000	0
60	2,3,4-trimethylhexane	0.9619	1.4861	6.0069	0	0	1.3611	0	2.2500	0	0
61	2,3,5-trimethylhexane	1.0072	0.9722	6.3333	0	0	2.2500	0	1.3611	0	0
62	2,4,4-trimethylhexane	1.0522	2.7361	2.2847	2.4722	0.2500	1.1111	2.0000	0	0.2500	0
63	3,3,4-trimethylhexane	1.0331	3.2083	1.8611	2.6111	0.1111	1.2500	1.2500	0	1.0000	0
64	2-methyl-3-ethylhexane	0.4950	3.0556	3.0347	0	1.3611	2.8611	0	1.0000	0	0
65	2-methyl-4-ethylhexane	0.4725	3.1944	2.8472	0	0.7500	4.2222	0	0.2500	0	0
66	3-methyl-3-ethylhexane	0.4272	4.8056	0	1.6111	1.9722	0	3.2500	0	0	0
67	3-methyl-4-ethylhexane	0.3786	3.9444	2.3333	0	0.4722	3.7500	0	1.0000	0	0
68	2,2,3,3-tetramethylpentane	2.0764	1.8333	0	6.6111	0	0	1.2500	0	0	1.0000
69	2,2,3,4-tetramethylpentane	1.9306	0	4.8333	3.4722	0	0	0	1.0000	1.2500	0
70	2,2,4,4-tetramethylpentane	2.0625	1.5000	0	6.6667	0	0	2.0000	0	0	0.2500
71	2,3,3,4-tetramethylpentane	1.8889	0	5.4444	3.0000	0	0	0	0.2500	2.0000	0
72	2,2-dimethyl-3-ethylpentane	1.1875	2.8889	1.2500	3.2222	0.2500	2.0000	0.5000	0	1.0000	0
73	2,3-dimethyl-3-ethylpentane	1.0069	3.1667	2.4722	2.0000	0.2500	0.5000	2.0000	0	1.0000	0
74	2,4-dimethyl-3-ethylpentane	1.0000	1.4444	5.9167	0	0	1.5000	0	2.2500	0	0

Table 2 (Continued)

no.	compound	m_{11}	m_{12}	m_{13}	m_{14}	m_{22}	m_{23}	m_{24}	m_{33}	m_{34}	m_{44}
75	3,3-diethylpentane	0.3750	5.3333	0	1.0000	1.5000	0	4.0000	0	0	0
76	decane	0.0123	3.0548	0	0	9.5015	0	0	0	0	0
77	2-methylnonane	0.2813	2.5150	2.0204	0	6.4983	1.4914	0	0	0	0
78	3-methylnonane	0.1471	3.4872	1.2778	0	5.5261	2.4636	0	0	0	0
79	4-methylnonane	0.1059	3.6972	1.1511	0	5.3161	2.6736	0	0	0	0
80	5-methylnonane	0.0956	3.7458	1.1250	0	5.2675	2.7222	0	0	0	0
81	2,2-dimethyloctane	0.8112	2.9378	0	3.0278	5.0347	0	1.4636	0	0	0
82	2,3-dimethyloctane	0.5408	2.3700	3.8178	0	3.6111	1.8872	0	1.0000	0	0
83	2,4-dimethyloctane	0.4558	2.8353	3.4236	0	2.6736	3.5747	0	0.2500	0	0
84	2,5-dimethyloctane	0.4333	2.9325	3.3264	0	2.5347	3.8525	0	0.1111	0	0
85	2,6-dimethyloctane	0.4575	2.7900	3.3978	0	2.6736	3.7622	0	0.0625	0	0
86	2,7-dimethyloctane	0.5816	1.8544	4.1111	0	3.6111	2.8472	0	0.0400	0	0
87	3,3-dimethyloctane	0.5482	4.1200	0	2.2900	4.0747	0	2.4236	0	0	0
88	3,4-dimethyloctane	0.3729	3.5175	2.9636	0	2.4636	3.0347	0	1.0000	0	0
89	3,5-dimethyloctane	0.3243	3.7953	2.6858	0	1.7136	4.5347	0	0.2500	0	0
90	3,6-dimethyloctane	0.3382	3.7050	2.7050	0	1.7622	4.6250	0	0.1111	0	0
91	4,4-dimethyloctane	0.4754	4.3786	0	2.1736	3.8872	0	2.6111	0	0	0
92	4,5-dimethyloctane	0.3365	3.7050	2.8472	0	2.2761	3.2222	0	1.0000	0	0
93	3-ethyloctane	0.1033	4.1842	0.5400	0	4.7883	3.4236	0	0	0	0
94	4-ethyloctane	0.0882	4.2989	0.4236	0	4.6719	3.6111	0	0	0	0
95	2,2,3-trimethylheptane	1.2067	2.4256	1.8125	3.2900	2.2500	1.3611	0.4236	0	1.0000	0
96	2,2,4-trimethylheptane	1.0833	2.9811	1.4444	3.1511	1.3611	2.2500	1.1736	0	0.2500	0
97	2,2,5-trimethylheptane	1.0644	2.9881	1.4375	3.1025	1.3611	2.2500	1.3125	0	0.1111	0
98	2,2,6-trimethylheptane	1.1667	2.1181	2.1200	3.0800	2.2500	1.3611	1.3611	0	0.0625	0
99	2,3,3-trimethylheptane	1.0800	2.6356	2.5400	2.5625	2.2500	0.4236	1.3611	0	1.0000	0
100	2,3,4-trimethylheptane	0.8664	1.9897	5.7969	0	1.0000	1.7847	0	2.2500	0	0
101	2,3,5-trimethylheptane	0.8214	2.2258	5.5122	0	0.2500	3.4236	0	1.3611	0	0
102	2,3,6-trimethylheptane	0.9133	1.4306	6.0975	0	1.0000	2.8611	0	1.1736	0	0
103	2,4,4-trimethylheptane	0.9306	3.2397	2.2622	2.3333	1.3611	1.1736	2.2500	0	0.2500	0
104	2,4,5-trimethylheptane	0.7953	2.3647	5.4219	0	0.1111	3.5625	0	1.3611	0	0
105	2,4,6-trimethylheptane	0.8611	1.7500	5.8267	0	0.2500	4.2222	0	0.5625	0	0
106	2,5,5-trimethylheptane	0.9378	3.1981	2.1650	2.3750	1.3611	1.3125	2.2500	0	0.1111	0
107	3,3,4-trimethylheptane	0.9272	3.7119	1.7222	2.5625	1.1736	1.5000	1.3611	0	1.0000	0
108	3,3,5-trimethylheptane	0.8561	3.9897	1.5347	2.4236	0.5625	2.1111	2.1111	0	0.2500	0
109	3,4,4-trimethylheptane	0.9011	3.7606	1.8125	2.4722	1.1736	1.3611	1.5000	0	1.0000	0
110	3,4,5-trimethylheptane	0.7397	2.9272	5.0694	0	0.0625	2.7222	0	2.2500	0	0
111	2-methyl-3-ethylheptane	0.4583	3.2642	2.9636	0	2.6736	3.0347	0	1.0000	0	0
112	2-methyl-4-ethylheptane	0.4256	3.4897	2.6858	0	1.9722	4.5347	0	0.2500	0	0
113	2-methyl-5-ethylheptane	0.4236	3.4517	2.7050	0	1.9722	4.6250	0	0.1111	0	0
114	3-methyl-3-ethylheptane	0.3803	5.1617	0	1.5625	3.3472	0	3.3611	0	0	0
115	3-methyl-4-ethylheptane	0.3214	4.2883	2.1458	0	1.6458	4.1111	0	1.0000	0	0
116	3-methyl-5-ethylheptane	0.3092	4.3406	2.0486	0	1.1250	5.3333	0	0.2500	0	0
117	4-methyl-3-ethylheptane	0.3056	4.3406	2.1458	0	1.5972	4.1111	0	1.0000	0	0
118	4-methyl-4-ethylheptane	0.3439	5.1494	0	1.4722	3.2569	0	3.5000	0	0	0
119	4-propylheptane	0.0833	4.3650	0.3333	0	4.6042	3.7500	0	0	0	0
120	4-isopropylheptane	0.4378	3.3994	2.8472	0	2.5347	3.2222	0	1.0000	0	0
121	2,2,3,3-tetramethylhexane	1.9117	2.4931	0	6.4236	1.0000	0	1.6111	0	0	1.0000
122	2,2,3,4-tetramethylhexane	1.6756	1.5486	3.9444	3.4236	0	1.2500	0.1111	1.0000	1.2500	0
123	2,2,3,5-tetramethylhexane	1.6983	1.0833	4.2708	3.3750	0	2.0000	0.2500	0.2500	1.1111	0
124	2,2,4,4-tetramethylhexane	1.7172	3.0486	0	5.8681	0.2500	0	3.1111	0	0	0.2500
125	2,2,4,5-tetramethylhexane	1.6497	1.2222	4.2708	3.2361	0	1.2500	1.0000	1.0000	0.3611	0
126	2,2,5,5-tetramethylhexane	1.8600	2.1667	0	6.3750	1.0000	0	2.5000	0	0	0.1111
127	2,3,3,4-tetramethylhexane	1.6078	1.5972	4.6458	2.8611	0	1.1111	0.2500	0.2500	2.0000	0
128	2,3,3,5-tetramethylhexane	1.6044	1.2222	4.9722	2.7222	0	1.2500	1.0000	0.1111	1.2500	0
129	2,3,4,4-tetramethylhexane	1.5592	1.7361	4.6458	2.7222	0	0.3611	1.0000	1.0000	1.2500	0
130	2,3,4,5-tetramethylhexane	1.4656	0	8.9167	0	0	0	0	3.6111	0	0
131	3,3,4,4-tetramethylhexane	1.6789	3.5694	0	5.7222	0.1111	0	2.5000	0	0	1.0000
132	2,2-dimethyl-3-ethylhexane	1.0975	3.3403	1.1111	3.1736	1.3611	2.2500	0.6111	0	1.0000	0
133	2,2-dimethyl-4-ethylhexane	1.0525	3.5694	0.8333	3.1250	0.7500	3.0000	1.2222	0	0.2500	0
134	2,3-dimethyl-3-ethylhexane	0.8908	3.6667	2.4236	1.8611	1.3611	0.6111	2.2500	0	1.0000	0
135	2,3-dimethyl-4-ethylhexane	0.8197	2.6944	5.0694	0	0.2500	2.7222	0	2.2500	0	0
136	2,4-dimethyl-3-ethylhexane	0.7936	2.8333	4.9792	0	0.1111	2.8611	0	2.2500	0	0
137	2,4-dimethyl-4-ethylhexane	0.8197	3.9444	2.2361	1.7222	0.7500	1.2222	3.0000	0	0.2500	0
138	2,5-dimethyl-3-ethylhexane	0.8650	2.1806	5.3958	0	0.2500	3.6111	0	1.3611	0	0
139	3,3-dimethyl-4-ethylhexane	0.8647	4.4167	1.1111	2.4722	0.4722	2.2500	1.5000	0	1.0000	0
140	3,4-dimethyl-3-ethylhexane	0.7744	4.5556	1.7222	1.8611	0.4722	1.5000	2.2500	0	1.0000	0
141	3,3-diethylhexane	0.3075	5.6250	0	0.8611	2.8333	0	4.2500	0	0	0
142	3,4-diethylhexane	0.2850	4.9444	1.4444	0	0.9444	5.0000	0	1.0000	0	0
143	2-methyl-3-isopropylhexane	0.9100	1.9444	5.6806	0	1.0000	1.9722	0	2.2500	0	0
144	2,2,3,3,4-pentamethylpentane	2.7361	0	2.8333	6.9722	0	0	0	0	1.2500	1.0000
145	2,2,3,4,4-pentamethylpentane	2.7292	0	2.5000	7.1667	0	0	0	0	2.0000	0.2500
146	2,2,3-trimethyl-3-ethylpentane	1.7431	3.3889	0	5.7222	0.2500	0	2.5000	0	0	1.0000
147	2,2,4-trimethyl-3-ethylpentane	1.6875	1.5556	3.9444	3.3333	0	1.2500	0.2500	1.0000	1.2500	0

Table 2 (Continued)

no.	compound	m_{11}	m_{12}	m_{13}	m_{14}	m_{22}	m_{23}	m_{24}	m_{33}	m_{34}	m_{44}
148	2,3,4-trimethyl-3-ethylpentane	1.5556	1.6944	5.1667	2.2500	0	0.5000	1.0000	0.2500	2.0000	0
149	2-methyl-3,3-diethylpentane	0.8125	4.3333	2.3333	1.2500	0.7500	0.7500	3.0000	0	1.0000	0
150	2,4-dimethyl-3-isopropylpentane	1.5000	0	8.8333	0	0	0	0	3.7500	0	0

Table 3. Distribution in Distances between Every Possible Pair of MEDVs

interval of distance	frequency(%)
0.00−0.05	0.00
0.05−0.50	0.40
0.50−1.50	2.17
1.50−2.50	5.73
2.50−3.50	9.70
3.50−4.50	17.58
4.50−5.50	20.47
5.50−6.50	17.05
6.50−7.50	10.20
7.50−8.50	6.95
8.50−9.50	5.59
9.50−10.50	2.68
10.50−11.50	0.91
11.50−12.50	0.49
12.50−13.50	0.04
13.50−14.50	0.02

where n is the number of samples used in creating the QSPR model of one property, $\bar{y}$ is the average value of n property data and y_i, and $\hat{y}_i$ is the experimental value and the calculated one for the examined property, respectively.

RESULTS AND DISCUSSION

Data Set for Thermodynamics and Physical Properties of 150 Alkanes. To build a property data set, 150 alkanes from C1 to C10 were selected. The data set includes 150 boiling points (BP);[34] 134 densities (D) at 25 °C, refraction indices (RI) at 25 °C, and heat capacities (HC) at 300 K[35]; 74 critical temperatures (CT) and critical pressures (CP); 68 surface tensions (ST) at 20 °C; 69 molar volumes (MV) at 20 °C, molar refractions (MR) at 20 °C, and heats of vaporization (HV) at 25 °C;[36] 44 heats of atomization (HA) at 25 °C; 54 standard heats of formation (HF) at 25 °C;[37] 62 heats of formation in liquid (HFL) at 25 °C; and 63 heats of formation in gas (HFG) at 25 °C[38] of the examined alkanes.

The MEDV of 150 Alkanes. Various conjunction relationships of the 150 alkanes were input into the program GITMED, and the MEDV for each alkane was calculated using the program.[33] The MEDV results are listed in Table 2. From Table 2, no two vectors are the same among 150 MEDVs of alkanes. All Euler's distances between every possible pair of vectors are larger than 0.07. The maximum among all 11 175 distances is 13.9381 and the minimum is 0.0731. The frequencies, the ratios of counting of vector pairs located in an interval of distance to all vector pairs (11 175), in different intervals are listed in Table 3, and the corresponding histogram is shown in Figure 2. This shows that the MEDVs have good discrimination ability for alkanes. The distances can be also used to perform similarity analysis. The longer the distance is, the smaller the similarity is.

QSPR Models. Taking 10 elements in the MEDV of the examined alkanes as 10 independent variables and one of 15 physical properties or thermodynamic functions as a dependent variable, various regression coefficients of eq 2A or 2B were calculated using MLR. It has been shown in our previous paper[28] that the logarithmic models (eq 2B) of some properties such as boiling point give better results than the corresponding general conventional models (eq 2A). In our present work, we used logarithmic models for six properties including boiling point (BP), density (D), refraction index (RI), critical temperature (CT), critical pressure (CP), and surface tension (ST). The six optimal values (opt) in the logarithmic models were obtained using a trial method, and they are 539.85 K, 867.00 g/cm^3, 1.4918, 756.15 K, 1.00 atm, and 36.00 dyn/cm.

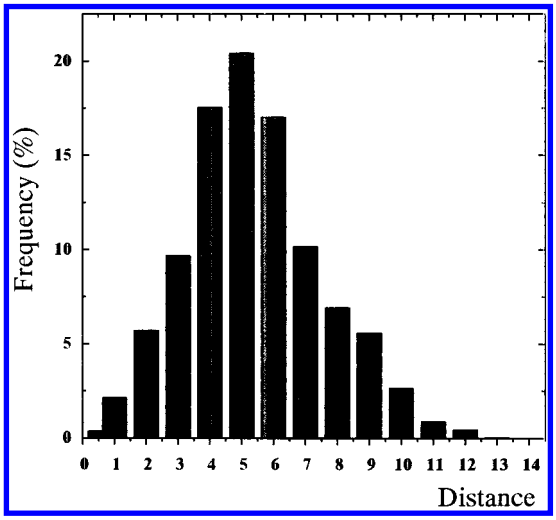

Figure 2. Histogram of the distribution in distances.

First, 15 conventional models that link the 15 physical properties or thermodynamic functions to the MEDV of alkanes and the six logarithmic models between the six physical properties and the MEDV were developed using MLR techniques. The resulting regression equations are listed in Table 4. To compare the estimation abilities of the 21 models for their physical properties or thermodynamic functions, two important statistical parameters, correlation coefficient (R) and root-mean-square error (rms) were also calculated and their results are listed in Table 5. From Table 5, the correlation coefficients of the 21 models are all more than 0.9840, which shows that there are good relationships between the MEDV and many physical properties or thermodynamic functions of alkanes. Here, it should be indicated that the logarithmic model of CP (Model 20 in Table 4) is different from the other five models because its optimal value is at atmospheric pressure and is smaller than the CP of the alkanes used to build the model.

Estimation of Properties. Second, the estimated values of the 15 properties were obtained using the models in Table 4. For most QSPR models, there are no remarkable estimation errors; i.e., the difference between experimental and estimated properties is in general less than 5%. However, there are several samples that have larger errors (>5%), and they are no. 2 (BP_{exp} = 184.55 K, ΔBP = 14.61 K), no. 3 (BP_{exp} = 231.05 K, ΔBP = 23.57 K) and no. 4 (BP_{exp} = 2272.65 K, ΔBP = 15.82 K) for the BP model; no. 8 (CP_{exp} = 31.57 atm, ΔCP = 1.82 atm), no. 42 (CP_{exp} = 23.60 atm,

Table 4. Regression Coefficients of 21 QSPR Models for Alkanes

no.	model	b_0	b_1	b_2	b_3	b_4	b_5	b_6	b_7	b_8	b_9	b_{10}
1	BP	107.0969	92.0674	62.2532	30.5024	7.8862	15.5087	−8.9157	−23.8692	−21.5509	−28.0297	−25.1267
2	D	428.4025	187.0574	72.2972	17.2120	−21.6334	7.9624	−18.2468	−31.9687	−27.9849	−29.6751	−18.3243
3	RI	1.2418	0.1033	0.0414	0.0109	−0.0107	0.0043	−0.0114	−0.0198	−0.0185	−0.0214	−0.0160
4	CT	−63.9766	383.3350	178.1941	59.9176	−24.0699	14.0586	−60.4930	−106.0804	−108.9363	−138.3903	−165.2422
5	CP	55.9774	−8.8881	−6.8370	−4.1841	−2.3144	−1.5760	1.4248	4.2134	4.8993	8.3069	10.2963
6	ST	−8.0247	21.0836	8.1885	1.8520	−2.6041	0.7341	−2.5815	−4.4614	−4.0070	−4.8351	−4.5786
7	MR	7.5273	4.5587	3.9832	3.3935	2.8327	3.0257	2.1516	1.2971	1.0167	−0.0761	−1.4648
8	MV	87.9867	−20.5235	1.4522	10.4434	16.0906	10.8251	12.7608	12.3088	10.1552	6.6783	−0.6295
9	HC	67.1121	6.4015	7.1611	11.0733	12.2341	15.2640	17.3995	18.2527	16.7543	14.2826	13.8325
10	E	1.2007	15.0368	5.6498	2.1246	−0.3124	3.0221	0.9032	−0.7917	−0.7610	−2.5156	−4.1701
11	HV	9.7352	2.9088	3.7084	2.7904	1.9695	3.1764	2.1694	1.5009	2.2958	2.4602	3.4795
12	HA	960.3331	1999.6646	1310.1407	913.5847	593.2357	762.9421	430.1958	152.8320	84.1203	−221.8696	−559.8767
13	HF	145.2684	−62.1157	−9.0173	13.8136	28.6326	14.1267	21.9915	26.8368	21.3816	20.9616	17.6950
14	HFL	24.8347	−2.3221	2.9425	4.9344	5.8831	4.0598	3.7893	3.3491	1.8043	0.3856	−1.9351
15	HFG	17.9408	2.1775	3.5851	4.4769	4.5742	3.2841	2.6097	1.9355	0.0494	−1.8555	−4.5691
16	ln(539.85 − BP)	6.0567	−0.1939	−0.1299	−0.0840	−0.0372	−0.1149	−0.0800	−0.0770	−0.0984	−0.1391	−0.2418
17	ln(867 − D)	6.5441	−0.9379	−0.3577	−0.0815	0.1198	−0.0517	0.0668	0.1109	0.0821	0.0341	−0.1366
18	ln(1.4918 − RI)	−0.9030	−0.9093	−0.3703	−0.1005	0.0965	−0.0471	0.0851	0.1440	0.1268	0.1163	−0.0242
19	ln(756.15 − CT)	6.4395	−0.3638	−0.2113	−0.1015	−0.0130	−0.0870	−0.0235	−0.0129	−0.0264	−0.0771	−0.1375
20	ln(CP − 1)	3.8723	−0.0269	−0.0882	−0.0969	−0.0981	−0.0664	−0.0309	0.0209	0.0443	0.1283	0.1629
21	ln(36 − ST)	3.9274	−0.8120	−0.3032	−0.0591	0.1136	−0.0524	0.0595	0.1090	0.0683	0.0562	−0.0411

Table 5. The R and rms of 21 QSPR Models

no.	n	R	rms	R^a	rms^a	no.	n	R	rms	R^a	rms^a	no.	n	R	rms	R^a	rms^a
1	150	0.9951	4.81	0.9790	9.92	8	69	0.9998	0.359	0.9973	1.261	15	63	0.9975	0.70	0.9924	1.22
2	134	0.9883	4.00	0.9851	4.51	9	134	0.9886	3.81	0.9857	4.25	16	150	0.9978	3.22	0.9671	12.38
3	134	0.9843	0.0024	0.9803	0.0027	10	134	0.9937	0.48	0.9921	0.54	17	134	0.9940	2.86	0.9925	3.20
4	74	0.9924	7.02	0.9786	11.71	11	69	0.9991	0.22	0.9982	0.32	18	134	0.9884	0.0021	0.9855	0.0023
5	74	0.9848	0.75	0.9567	1.25	12	44	0.9998	29.98	0.9996	47.39	19	74	0.9956	5.30	0.9813	10.96
6	68	0.9880	0.30	0.9812	0.37	13	54	0.9960	2.58	0.9912	3.85	20	74	0.9909	0.58	0.9793	0.87
7	69	0.9999	0.0643	0.9996	0.1491	14	62	0.9977	0.72	0.9961	0.94	21	68	0.9907	0.26	0.9828	0.35

[a] The results of cross-validation.

$\Delta CP = -1.27$ atm), no. 49 ($CP_{exp} = 23.70$ atm, $\Delta CP = -1.51$ atm), no. 65 ($CP_{exp} = 25.56$ atm, $\Delta CP = -1.48$ atm), no. 67 ($CP_{exp} = 23.59$ atm, $\Delta CP = 1.79$ atm), no. 68 ($CP_{exp} = 27.04$ atm, $\Delta CP = -1.79$ atm), no. 70 ($CP_{exp} = 24.58$ atm, $\Delta CP = -1.62$ atm) and no. 75 ($CP_{exp} = 26.94$ atm, $\Delta CP = 1.42$ atm) for the CP model; no. 6 ($ST_{exp} = 16.00$ dyn/cm, $\Delta ST = 1.24$ dyn/cm) and no. 7 ($ST_{exp} = 15.00$ dyn/cm, $\Delta ST = 0.80$ dyn/cm) for the ST model; no. 146 ($HC_{exp} = 223.70$ J·K^{-1}·mol^{-1}, $\Delta HC = 12.12$ J·K^{-1}·mol^{-1}) and no. 149 ($HC_{exp} = 224.80$ J·K^{-1}·mol^{-1}, $\Delta HC = 13.21$ J·K^{-1}·mol^{-1}) for the HC model; no. 8 ($BP_{exp} = 282.65$ K, $\Delta BP = -17.85$ K) for the logarithmic models of BP; no. 2 ($CT_{exp} = 305.42$ K, $\Delta CT = 15.58$ K) and no. 8 ($CT_{exp} = 433.75$ K, $\Delta CT = -21.97$ K) for the logarithmic models of CT; no. 40 ($CP_{exp} = 24.50$ atm, $\Delta CP = 1.85$ atm), no. 65 ($CP_{exp} = 25.56$ atm, $\Delta CP = -1.62$ atm), no. 67 ($CP_{exp} = 23.59$ atm, $\Delta CP = 1.58$ atm) and no. 68 ($CP_{exp} = 27.04$ atm, $\Delta CP = -1.61$ atm) for the logarithmic models of CP; no. 6 ($ST_{exp} = 16.00$ dyn/cm, $\Delta ST = 1.21$ dyn/cm) for the logarithmic models of ST. The estimated results using the six logarithmic models are better than those obtained using the six conventional models.

Cross-Validation Testing. An excellent QSPR model should have not only an good estimation ability for any internal sample, but should also have a good prediction ability for an external sample. Although it has been proved that the above models have good estimation abilities for 15 physical properties or thermodynamic functions except for several data having larger estimation errors, the prediction abilities for the external samples have to be further tested. The most usual method to prove that a model has excellent prediction ability is a cross-validation (CV) method. In the present paper, $n - 1$ samples from a total data set are used to construct a calibration set and to build a QSPR model between the MEDV and the examined physical property or thermodynamic function using MLR. The property of the sample is then predicted using the one sample that was left out of the data set. The procedure above is repeated until every sample in the total data set is used for a prediction. Then the prediction values are compared to the experimental values and the R and rms between them are calculated. It should be noted that the calculations are similar to single variable regression or linear regression and are performed between the n experimental values and n times of predicted values obtained using n cross-validation models. The results for the CV methods are also listed in Table 5. The prediction results obtained using the CV technique show that there are indeed several samples that have large errors (>5%). They are no. 1 ($BP_{exp} = 109.15$, $\Delta BP = -96.38$), no. 2 ($BP_{exp} = 184.55$, $\Delta BP = 39.75$), no. 3 ($BP_{exp} = 231.05$, $\Delta BP = 26.41$), and no. 4 ($BP_{exp} = 2272.65$, $\Delta BP = 17.67$) for the BP (K); no. 2 ($CT_{exp} = 305.42$, $\Delta CT = 69.11$), no. 3 ($CT_{exp} = 369.95$, $\Delta CT = 25.79$), and no. 8 ($CT_{exp} = 433.75$, $\Delta CT = -28.45$) for the CT (K); no. 2 ($CP_{exp} = 48.20$, $\Delta CP = -5.51$), no. 3 ($CP_{exp} = 42.01$, $\Delta CP = -2.72$), no. 8 ($CP_{exp} = 31.57$, $\Delta CP = 2.72$), no. 40 ($CP_{exp} = 24.50$, $\Delta CP = 4.41$), no. 42 ($CP_{exp} = 23.60$, $\Delta CP = -1.44$), no. 49 ($CP_{exp} = 23.70$, $\Delta CP = -1.75$), no. 65 ($CP_{exp} = 25.56$, $\Delta CP = -1.64$), no. 67 ($CP_{exp} = 23.59$, $\Delta CP = 2.11$), no. 68 ($CP_{exp} = 27.04$, $\Delta CP = -3.74$), no. 70 ($CP_{exp} = 24.58$, $\Delta CP = -2.36$) and no. 75 ($CP_{exp} = 26.94$, $\Delta CP = 2.17$) for the CP (atm); no. 6 ($ST_{exp} = 16.00$, $\Delta ST = 1.51$) and no. 7 ($ST_{exp} = 15.00$, $\Delta ST =$

Table 6. Experimental and Estimated Properties

(A) Experimental and Estimated (Model 16) Boiling Points for 150 Alkanes

no.	BP^0	BP^1	no.	BP^0	BP^1	no.	BP^0	BP^1	no.	BP^0	BP^1	no.	BP^0	BP^1	no.	BP^0	BP^1
1	109.15	112.90	26	390.85	393.21	51	413.25	414.38	76	447.27	443.73	101	430.15	428.94	126	410.61	412.99
2	184.55	188.14	27	379.95	380.86	52	409.15	409.62	77	440.15	436.34	102	428.85	427.43	127	437.74	437.37
3	231.05	226.14	28	388.75	389.74	53	408.35	412.24	78	440.95	436.74	103	426.15	427.65	128	426.15	429.25
4	272.65	270.63	29	382.55	384.14	54	416.15	418.13	79	438.85	436.88	104	430.15	429.00	129	435.35	434.31
5	261.45	252.93	30	382.15	382.54	55	414.35	418.42	80	438.25	436.92	105	417.95	424.14	130	434.15	433.35
6	309.25	311.14	31	385.15	386.31	56	404.85	409.16	81	428.15	428.37	106	425.95	425.52	131	443.65	439.61
7	300.95	294.84	32	390.85	390.18	57	399.65	400.23	82	437.46	434.33	107	437.15	434.64	132	432.15	432.51
8	282.65	264.80	33	391.65	394.55	58	397.15	397.96	83	426.15	430.49	108	428.83	427.40	133	420.15	424.54
9	342.15	346.57	34	383.15	383.58	59	410.85	413.26	84	429.95	429.69	109	437.15	435.17	134	442.15	438.64
10	333.45	332.26	35	372.35	372.51	60	412.15	413.09	85	431.69	429.26	110	437.15	434.12	135	437.15	434.83
11	336.45	332.75	36	387.85	387.73	61	404.45	407.01	86	433.02	428.69	111	439.15	435.63	136	437.15	434.89
12	322.85	313.66	37	386.55	388.39	62	399.65	404.62	87	434.35	432.60	112	433.15	431.94	137	431.15	431.67
13	331.15	328.16	38	388.75	390.92	63	413.65	413.63	88	439.15	434.81	113	432.85	430.84	138	430.15	429.80
14	371.55	377.05	39	391.35	391.47	64	411.15	415.23	89	433.15	430.89	114	436.95	439.27	139	438.15	436.18
15	363.15	364.79	40	379.65	383.67	65	406.95	410.51	90	433.15	429.98	115	440.15	436.22	140	443.15	438.93
16	365.15	365.29	41	423.92	425.10	66	413.75	416.76	91	430.65	433.45	116	431.45	432.04	141	439.45	442.18
17	352.35	350.25	42	415.95	416.32	67	413.55	415.59	92	435.25	434.91	117	440.15	436.03	142	435.15	437.23
18	362.95	361.39	43	416.95	416.77	68	413.42	414.40	93	439.15	437.98	118	440.15	438.09	143	436.15	434.59
19	353.65	354.28	44	415.55	416.88	69	406.15	408.91	94	436.79	438.36	119	433.15	438.71	144	439.20	439.07
20	359.25	355.71	45	405.85	406.65	70	395.85	391.53	95	431.15	430.59	120	433.15	435.92	145	432.44	428.58
21	366.65	366.56	46	413.65	413.89	71	414.65	416.07	96	420.85	423.19	121	431.15	436.06	146	441.15	440.11
22	354.05	352.48	47	406.65	409.26	72	406.98	410.83	97	421.15	421.57	122	428.05	430.89	147	428.45	432.03
23	398.85	403.05	48	409.15	408.23	73	414.75	417.59	98	421.35	420.55	123	421.55	424.97	148	442.59	440.63
24	390.75	392.64	49	408.35	407.41	74	409.88	413.79	99	433.25	434.23	124	426.45	420.67	149	447.15	442.58
25	391.15	393.13	50	410.45	411.53	75	419.35	421.49	100	436.15	433.76	125	421.35	421.55	150	430.19	434.76

(B) Experimental and Estimated (Model 17) Densities for 134 Alkanes

no.	D^0	D^1	no.	D^0	D^1	no.	D^0	D^1	no.	D^0	D^1	no.	D^0	D^1	no.	D^0	D^1
10	648.52	657.12	33	709.45	708.67	57	711.80	712.53	85	723.60	724.68	108	739.00	741.31	131	778.90	775.78
11	659.76	666.34	34	712.03	710.98	58	703.20	702.06	86	720.20	717.56	109	753.50	753.38	132	744.70	746.53
12	644.46	645.04	35	687.84	687.62	59	733.50	734.64	87	735.10	734.21	110	751.90	751.06	133	730.20	733.74
13	657.02	659.98	36	722.30	719.34	60	735.10	733.23	88	741.80	739.03	111	739.80	739.07	134	759.90	759.61
14	679.50	683.77	37	715.09	712.16	61	717.90	718.99	89	732.90	732.97	112	732.20	732.85	135	751.60	751.22
15	674.34	676.23	38	715.20	713.15	62	720.05	721.51	90	732.90	731.65	113	731.80	731.70	137	751.40	748.79
16	682.88	684.87	39	723.54	721.62	63	741.40	740.64	91	731.20	735.23	114	746.30	753.93	138	736.80	738.91
17	669.48	668.67	40	721.70	724.17	64	729.00	726.93	92	743.20	739.18	115	746.60	744.86	139	759.80	758.68
18	690.81	688.69	42	709.60	708.07	65	724.20	720.10	93	735.90	734.37	116	736.80	738.90	140	759.60	764.47
19	668.23	671.68	43	716.70	715.25	66	736.00	735.90	94	734.30	734.22	117	746.80	745.02	141	757.50	760.13
20	689.16	687.52	44	716.30	715.44	67	738.00	733.27	95	738.50	739.66	118	747.20	748.40	142	747.20	750.55
21	693.92	693.36	45	706.60	704.38	68	752.97	753.11	96	725.70	727.21	119	732.10	734.07	143	743.60	745.90
22	685.64	683.85	46	722.00	719.89	69	735.22	735.34	97	728.10	724.30	120	735.40	739.06	144	776.75	778.00
23	698.54	699.30	47	711.50	713.15	70	715.61	709.45	98	723.80	716.17	121	760.89	765.55	145	763.61	759.92
24	693.87	693.07	48	713.60	711.60	71	751.11	748.26	99	748.80	747.25	122	751.30	753.95	146	778.00	776.03
25	701.73	700.92	49	704.50	703.59	72	731.00	733.87	100	748.50	745.57	123	733.60	740.57	147	753.10	754.97
26	700.71	701.15	50	721.60	720.99	73	750.80	747.73	101	745.10	738.56	124	742.40	740.00	148	773.50	771.38
27	691.11	687.83	51	727.50	726.72	74	734.10	733.78	102	734.70	730.77	125	731.60	734.31	149	775.50	770.49
28	708.16	705.40	52	716.60	719.89	75	749.92	749.03	103	734.60	736.20	126	714.80	718.74	150	754.57	754.28
29	696.17	697.76	53	718.30	721.92	81	720.80	718.97	104	737.30	738.74	127	765.60	765.55			
30	689.37	688.20	54	722.50	722.16	82	734.40	732.80	105	719.00	725.74	128	744.90	749.19			
31	705.95	705.89	55	722.30	722.16	83	722.60	726.63	106	736.20	732.81	129	758.60	760.53			
32	715.15	712.72	56	725.70	726.46	84	726.40	725.42	107	752.70	752.81	130	745.60	752.68			

(C) Experimental and Estimated (Model 7) Molar Refraction for 69 Alkanes

no.	MR^0	MR^1	no.	MR^0	MR^1	no.	MR^0	MR^1	no.	MR^0	MR^1	no.	MR^0	MR^1
6	25.2656	25.4630	20	34.3323	34.2447	34	38.9249	38.8412	49	43.9258	43.9075	63	43.3407	43.2991
7	25.2923	25.4415	21	34.2827	34.2563	35	39.2617	39.2496	50	43.6870	43.6550	64	43.6550	43.5439
8	25.7243	25.6961	22	34.3736	34.2957	36	38.7617	38.6851	51	43.5473	43.5388	65	43.6472	43.6749
9	29.9066	29.9767	23	39.1922	39.1633	37	38.8681	38.8254	52	43.6378	43.6702	66	43.2680	43.3629
10	29.9459	29.9716	24	39.2316	39.1959	38	38.8362	38.8000	53	43.6022	43.6680	67	43.3746	43.3963
11	29.8016	29.8179	25	39.1001	39.0643	39	38.7171	38.6117	54	43.6420	43.6275	68	43.2147	43.1791
12	29.9347	29.9396	26	39.1174	39.0708	41	43.8423	43.8166	55	43.4907	43.6447	69	43.4359	43.4873
13	29.8014	29.8165	27	39.2525	39.2251	42	43.8795	43.8613	56	43.6226	43.5958	70	43.8747	44.0171
14	34.5504	34.5472	28	38.9808	38.9532	43	43.7296	43.7429	57	43.7638	43.8506	71	43.2016	43.2137
15	34.5908	34.5631	29	39.1300	39.0911	44	43.7687	43.7649	58	43.9356	43.9756	72	43.4571	43.4492
16	34.4597	34.4159	30	39.2596	39.2292	45	43.9138	43.9204	59	43.4347	43.4458	73	42.9542	43.1360
17	34.6166	34.5549	31	39.0087	38.9279	46	43.6269	43.6640	60	43.3917	43.4320	74	43.4037	43.4324
18	34.3237	34.2773	32	38.8453	38.8060	47	43.7393	43.8082	61	43.6474	43.7080	75	43.1134	43.0399
19	34.6192	34.5688	33	38.9441	38.9219	48	43.8484	43.7928	62	43.6598	43.7006			

Table 6 (Continued)

D. Experimental and Estimated (Model 18) Refraction Indices for 134 Alkanes

no.	RI^0	RI^1	no.	RI^0	RI^1	no.	RI^0	RI^1	no.	RI^0	RI^1	no.	RI^0	RI^1	no.	RI^0	RI^1
10	1.3687	1.3726	33	1.3992	1.3984	57	1.4010	1.4024	85	1.4084	1.4090	108	1.4170	1.4170	131	1.4368	1.4350
11	1.3739	1.3767	34	1.4007	1.3997	58	1.3973	1.3979	86	1.4062	1.4059	109	1.4235	1.4222	132	1.4174	1.4184
12	1.3660	1.3667	35	1.3890	1.3897	59	1.4119	1.4123	87	1.4142	1.4137	110	1.4229	1.4215	133	1.4107	1.4128
13	1.3723	1.3738	36	1.4052	1.4038	60	1.4120	1.4122	88	1.4159	1.4155	111	1.4151	1.4150	134	1.4247	1.4250
14	1.3851	1.3864	37	1.4020	1.4012	61	1.4037	1.4056	89	1.4115	1.4126	112	1.4114	1.4119	135	1.4203	1.4212
15	1.3823	1.3830	38	1.4017	1.4009	62	1.4052	1.4067	90	1.4115	1.4121	113	1.4111	1.4116	137	1.4202	1.4203
16	1.3861	1.3868	39	1.4055	1.4052	63	1.4154	1.4151	91	1.4122	1.4140	114	1.4185	1.4235	138	1.4232	1.4153
17	1.3800	1.3795	40	1.4057	1.4078	64	1.4091	1.4083	92	1.4167	1.4155	115	1.4183	1.4175	139	1.4246	1.4243
18	1.3895	1.3887	42	1.4008	1.4002	65	1.4054	1.4051	93	1.4136	1.4125	116	1.4141	1.4149	140	1.4244	1.4273
19	1.3788	1.3810	43	1.4040	1.4033	66	1.4134	1.4130	94	1.4131	1.4122	117	1.4184	1.4177	141	1.4235	1.4249
20	1.3884	1.3882	44	1.4041	1.4033	67	1.4128	1.4112	95	1.4145	1.4157	118	1.4187	1.4197	142	1.4167	1.4197
21	1.3971	1.3902	45	1.3995	1.3988	68	1.4214	1.4230	96	1.4092	1.4103	119	1.4113	1.4119	143	1.4172	1.4186
22	1.3869	1.3854	46	1.4064	1.4057	69	1.4125	1.4127	97	1.4101	1.4091	120	1.4132	1.4148	144	1.4341	1.4357
23	1.3951	1.3947	47	1.4011	1.4025	70	1.4046	1.4018	98	1.4178	1.4056	121	1.4260	1.4300	145	1.4281	1.4258
24	1.3926	1.3921	48	1.4015	1.4019	71	1.4200	1.4185	99	1.4202	1.4195	122	1.4193	1.4226	146	1.4397	1.4349
25	1.3961	1.3955	49	1.3985	1.3984	72	1.4101	1.4114	100	1.4195	1.4190	123	1.4119	1.4164	147	1.4199	1.4228
26	1.3955	1.3955	50	1.4063	1.4064	73	1.4197	1.4184	101	1.4169	1.4157	124	1.4185	1.4173	148	1.4310	1.4307
27	1.3910	1.3898	51	1.4091	1.4087	74	1.4115	1.4120	102	1.4131	1.4122	125	1.4132	1.4140	149	1.4320	1.4300
28	1.3988	1.3978	52	1.4046	1.4056	75	1.4184	1.4188	103	1.4143	1.4147	126	1.4055	1.4073	150	1.4246	1.4232
29	1.3929	1.3942	53	1.4053	1.4067	81	1.4060	1.4066	104	1.4160	1.4157	127	1.4298	1.4280			
30	1.3900	1.3901	54	1.4070	1.4058	82	1.4127	1.4128	105	1.4071	1.4098	128	1.4196	1.4205			
31	1.3978	1.3981	55	1.4067	1.4056	83	1.4069	1.4098	106	1.4149	1.4132	129	1.4267	1.4260			
32	1.4018	1.4011	56	1.4082	1.4083	84	1.4089	1.4093	107	1.4236	1.4220	130	1.4204	1.4228			

(E) Experimental and Estimated (Model 19) Critical Temperatures for 74 Alkanes

no.	CT^0	CT^1	no.	CT^0	CT^1	no.	CT^0	CT^1	no.	CT^0	CT^1	no.	CT^0	CT^1	no.	CT^0	CT^1
2	305.42	321.00	15	531.05	531.27	28	566.15	565.13	41	595.15	592.19	54	591.15	591.35	67	585.45	596.07
3	369.95	381.51	16	535.55	535.24	29	555.15	557.94	42	588.15	585.72	55	591.45	591.48	68	607.65	599.02
4	425.16	431.15	17	520.85	520.63	30	552.15	553.02	43	591.15	588.95	56	591.25	592.41	69	592.75	595.63
5	408.13	404.71	18	537.75	535.30	31	563.99	566.35	44	591.45	589.40	57	574.15	579.99	70	574.75	570.23
6	469.77	473.05	19	520.25	523.30	32	571.15	568.51	45	575.15	580.32	58	569.75	574.34	71	607.65	607.79
7	460.95	457.65	20	536.15	534.02	33	565.15	566.71	46	588.15	590.45	59	599.25	600.38	72	595.75	596.04
8	433.75	411.78	21	540.75	538.15	34	567.15	565.29	47	579.15	584.53	60	597.35	596.31	73	611.75	609.12
9	507.85	509.22	22	531.45	527.71	35	544.30	547.51	48	580.95	583.05	61	582.55	586.17	74	597.35	596.17
10	498.05	497.48	23	569.35	568.17	36	576.15	573.26	49	579.15	579.31	62	582.25	588.57	75	615.95	610.51
11	504.35	501.57	24	561.15	560.42	37	568.15	567.40	50	587.15	592.42	63	603.75	603.14			
12	489.35	480.14	25	565.15	564.03	38	568.15	568.00	51	595.85	593.81	64	595.85	593.20			
13	500.25	495.85	26	563.15	564.39	39	578.15	576.66	52	585.45	587.38	65	603.45	586.74			
14	540.16	540.70	27	552.15	553.05	40	543.95	556.84	53	590.95	593.92	66	600.35	602.57			

(F) Experimental and Estimated (Model 20) Critical Pressures for 74 Alkanes

no.	CP^0	CP^1	no.	CP^0	CP^1	no.	CP^0	CP^1	no.	CP^0	CP^1	no.	CP^0	CP^1	no.	CP^0	CP^1
2	48.20	47.78	15	27.20	27.50	28	26.60	26.30	41	22.74	22.64	54	23.98	23.82	67	23.59	25.17
3	42.01	41.01	16	28.10	28.15	29	25.80	25.65	42	23.60	22.60	55	23.98	23.89	68	27.04	25.43
4	37.47	36.96	17	28.40	28.00	30	25.00	24.97	43	23.70	23.13	56	25.07	24.95	69	25.66	25.94
5	36.00	36.22	18	29.20	28.96	31	27.20	26.87	44	23.06	23.18	57	23.39	23.84	70	24.58	23.50
6	33.31	33.49	19	27.40	27.65	32	27.40	26.93	45	22.80	23.05	58	22.41	23.12	71	26.85	27.25
7	32.90	33.41	20	30.00	29.44	33	25.74	26.28	46	23.79	23.84	59	25.56	25.76	72	25.96	25.75
8	31.57	32.18	21	28.60	28.90	34	28.20	27.44	47	22.70	23.30	60	25.46	25.31	73	26.94	27.27
9	29.92	30.38	22	29.75	29.40	35	25.50	25.66	48	22.70	23.16	61	23.49	24.03	74	25.46	25.49
10	29.95	30.33	23	24.64	24.97	36	29.00	28.24	49	23.70	22.60	62	23.79	24.61	75	26.94	27.51
11	30.83	30.99	24	24.80	24.93	37	27.60	27.24	50	24.19	24.39	63	26.45	26.37			
12	30.67	30.70	25	25.60	25.52	38	27.40	27.05	51	24.77	24.45	64	24.77	24.59			
13	30.99	31.17	26	25.60	25.58	39	28.90	28.38	52	23.59	23.80	65	25.56	23.94			
14	27.01	27.55	27	25.60	25.42	40	24.50	26.35	53	24.18	24.52	66	25.66	25.92			

(G) Experimental and Estimated (Model 21) Surface Tensions for 68 Alkanes

no.	ST^0	ST^1	no.	ST^0	ST^1	no.	ST^0	ST^1	no.	ST^0	ST^1	no.	ST^0	ST^1	no.	ST^0	ST^1
6	16.00	17.21	19	18.15	18.03	31	20.63	20.70	44	22.34	22.26	56	21.86	22.03	68	23.38	23.42
7	15.00	15.60	20	19.59	19.14	32	21.64	21.41	45	20.80	20.99	57	20.51	20.91	69	21.98	22.44
9	18.42	18.84	21	20.44	20.23	33	21.51	21.57	46	22.34	22.20	58	20.04	20.15	70	20.37	20.15
10	17.38	17.42	22	18.76	18.44	34	20.67	20.64	47	21.30	21.51	59	22.41	22.57	71	23.31	23.29
11	18.12	18.04	23	21.76	21.62	35	18.77	18.84	48	21.30	21.38	60	22.80	22.86	72	22.38	22.59
12	16.30	16.01	24	20.60	20.49	36	21.56	21.20	49	20.83	20.82	61	21.27	21.60	73	23.87	23.55
13	17.37	17.21	25	21.17	21.00	37	21.14	21.11	50	22.01	22.05	62	21.17	21.50	74	22.80	22.92
14	20.26	20.31	26	21.00	21.00	38	21.52	21.48	51	22.80	22.66	63	23.27	23.02	75	23.75	24.10
15	19.29	19.04	27	19.60	19.53	39	21.99	21.82	52	21.77	21.99	64	22.80	22.71			
16	19.79	19.61	28	20.99	20.90	41	22.92	22.82	53	22.01	22.09	65	21.77	22.04			
17	18.02	17.90	29	20.05	20.15	42	21.88	21.81	54	22.81	22.77	66	23.22	23.10			
18	19.96	19.46	30	19.73	19.45	43	22.34	22.27	55	22.81	22.76	67	23.27	23.16			

Table 6 (Continued)

(H) Experimental and Estimated (Model 8) Molar Volumes for 69 Alkanes

no.	MV^0	MV^1	no.	MV^0	MV^1	no.	MV^0	MV^1	no.	MV^0	MV^1	no.	MV^0	MV^1
6	115.205	115.014	20	144.530	144.682	34	159.526	159.410	49	180.914	181.078	63	172.055	172.111
7	116.426	116.732	21	143.517	143.697	35	165.083	164.536	50	176.897	177.051	64	175.445	175.357
8	122.074	121.564	22	145.191	145.495	36	157.292	157.673	51	175.349	175.307	65	177.386	177.199
9	130.688	130.391	23	162.592	162.245	37	158.852	158.846	52	177.386	177.149	66	173.077	173.474
10	131.933	131.978	24	163.663	163.690	38	158.794	158.729	53	176.897	177.147	67	172.844	173.432
11	129.717	129.990	25	161.832	161.869	39	157.026	156.916	54	176.410	176.502	68	169.495	169.167
12	132.744	132.898	26	162.105	161.932	41	178.713	178.547	55	175.685	176.691	69	173.557	173.213
13	130.240	130.976	27	164.285	164.341	42	179.773	179.926	56	175.878	175.739	70	178.256	179.567
14	146.540	146.168	28	160.395	160.730	43	177.952	178.172	57	179.220	178.878	71	169.928	170.245
15	147.656	147.686	29	163.093	162.635	44	178.150	178.339	58	181.346	181.192	72	174.537	173.772
16	145.821	145.761	30	164.697	164.778	45	180.507	180.500	59	173.780	174.038	73	170.093	170.302
17	148.695	148.405	31	160.879	160.715	46	176.653	177.065	60	173.498	173.353	74	173.804	173.341
18	144.153	144.628	32	158.814	158.805	47	179.120	179.033	61	177.656	177.402	75	170.185	169.599
19	148.949	148.521	33	160.072	159.994	48	179.371	179.189	62	177.787	177.176			

(I) Experimental and Estimated (Model 9) Heat Capacities for 134 Alkanes

no.	HC^0	HC^1	no.	HC^0	HC^1	no.	HC^0	HC^1	no.	HC^0	HC^1	no.	HC^0	HC^1	no.	HC^0	HC^1
10	143.01	144.03	33	190.58	189.69	57	210.70	211.67	85	231.90	234.96	108	234.10	235.23	131	238.00	234.59
11	140.88	143.65	34	186.77	186.81	58	209.10	211.85	86	233.20	234.97	109	235.60	233.38	132	227.70	234.55
12	142.26	144.59	35	189.45	189.35	59	213.30	210.04	87	237.10	234.57	110	235.10	234.96	133	236.10	236.39
13	142.21	145.28	36	188.20	187.16	60	214.00	211.81	88	229.30	234.67	111	238.50	236.60	134	238.20	235.44
14	166.00	165.10	37	192.72	189.35	61	212.50	212.61	89	238.30	235.35	112	243.40	237.76	135	243.00	236.67
15	165.40	165.90	38	193.05	189.56	62	213.50	212.21	90	229.60	234.99	113	234.30	236.93	137	235.00	237.48
16	164.50	165.66	39	189.07	189.69	63	210.50	209.80	91	239.30	235.10	114	236.20	238.07	138	240.80	237.47
17	167.70	165.96	40	188.28	188.70	64	216.10	213.08	92	230.10	234.89	115	236.20	237.05	139	228.20	234.84
18	161.80	166.22	42	210.90	211.26	65	219.70	213.64	93	235.80	236.37	116	240.90	237.02	140	235.50	235.19
19	171.70	167.28	43	209.70	211.18	66	214.10	213.40	94	236.50	237.30	117	238.60	236.58	141	242.50	240.72
20	166.70	165.94	44	210.40	211.40	67	215.20	212.83	95	232.50	232.57	118	239.20	237.80	142	246.90	238.51
21	166.80	166.52	45	212.40	210.90	68	213.34	211.06	96	234.70	234.86	119	237.70	238.12	143	231.80	237.04
22	164.20	165.33	46	207.70	211.40	69	208.50	210.08	97	230.50	234.67	120	239.20	237.29	144	234.30	232.99
23	188.70	187.79	47	217.10	212.21	70	215.77	212.58	98	234.80	234.67	121	238.20	234.29	145	234.20	231.97
24	188.20	188.38	48	208.20	211.95	71	219.50	208.95	99	235.10	233.22	122	229.40	232.88	146	223.70	235.82
25	186.82	188.23	49	210.40	211.98	72	205.00	210.69	100	237.60	235.11	123	235.80	233.74	147	227.30	234.43
26	188.03	188.35	50	214.00	211.39	73	213.40	211.38	101	233.90	235.54	124	239.20	235.79	148	229.00	233.65
27	189.33	188.18	51	206.80	211.37	74	209.00	213.17	102	228.50	235.43	125	229.20	235.22	149	224.80	238.01
28	185.18	188.57	52	214.60	211.93	75	217.86	215.85	103	238.90	235.70	126	229.80	234.96	150	234.50	237.36
29	193.35	189.26	53	217.20	211.71	81	235.10	233.95	104	234.10	235.66	127	241.50	231.94			
30	186.52	189.37	54	213.00	212.96	82	230.50	234.53	105	246.30	236.38	128	234.00	234.21			
31	191.96	188.48	55	214.30	213.56	83	239.40	235.44	106	234.20	235.32	129	231.80	233.42			
32	182.72	188.32	56	209.90	209.50	84	231.80	235.30	107	233.60	233.19	130	243.10	235.73			

(J) Experimental and Estimated (Model 10) Enthalpies for 134 Alkanes

no.	E^0	E^1	no.	E^0	E^1	no.	E^0	E^1	no.	E^0	E^1	no.	E^0	E^1	no.	E^0	E^1
10	26.61	26.62	33	36.07	35.82	57	36.61	36.60	85	42.09	42.49	108	40.46	40.42	131	39.87	39.01
11	26.32	26.61	34	32.13	32.31	58	36.86	36.60	86	42.58	42.61	109	40.08	40.15	132	40.50	41.09
12	25.40	25.57	35	32.55	32.37	59	36.28	36.06	87	42.80	42.40	110	41.14	40.57	133	41.92	41.37
13	24.77	25.26	36	32.17	31.96	60	36.86	36.34	88	41.80	42.40	111	43.30	42.89	134	40.70	40.25
14	33.56	33.37	37	32.55	32.20	61	36.02	36.29	89	42.47	42.31	112	43.64	42.89	135	42.43	41.02
15	31.21	31.05	38	34.31	33.82	62	36.44	36.11	90	41.63	42.38	113	42.93	42.87	137	40.29	40.39
16	30.71	30.95	39	33.26	33.33	63	35.98	35.96	91	42.30	42.09	114	42.13	43.05	138	41.34	40.97
17	29.50	29.54	40	31.84	32.28	64	38.70	38.29	92	41.51	42.27	115	42.47	42.75	139	39.92	40.50
18	28.62	29.27	42	40.42	40.24	65	39.25	38.29	93	45.31	45.10	116	43.35	42.75	140	40.42	40.15
19	29.58	29.19	43	39.92	40.09	66	37.36	37.66	94	45.10	45.10	117	42.51	42.66	141	42.43	42.53
20	29.33	29.18	44	39.71	39.95	67	38.07	38.19	95	41.30	41.05	118	41.46	42.08	142	43.60	43.10
21	31.84	31.31	45	38.83	38.47	68	35.86	35.56	96	41.05	41.00	119	44.85	45.12	143	40.46	41.03
22	28.28	28.50	46	37.82	38.07	69	35.06	35.51	97	40.50	41.00	120	43.10	42.85	144	38.62	38.87
23	38.12	38.00	47	38.16	37.88	70	36.44	35.98	98	40.96	41.05	121	40.00	39.60	145	38.81	39.24
24	35.82	35.61	48	37.53	37.92	71	36.23	35.01	99	41.00	40.52	122	39.25	39.59	146	38.41	39.38
25	35.31	35.47	49	37.99	38.01	72	36.15	36.68	100	40.90	40.71	123	39.54	39.50	147	38.87	39.73
26	35.06	35.38	50	38.20	37.79	73	36.61	35.97	101	40.12	40.65	124	40.29	39.66	148	38.58	38.88
27	34.23	33.92	51	37.02	37.84	74	36.07	36.61	102	39.75	40.68	125	38.83	39.64	149	39.25	40.52
28	33.05	33.56	52	38.07	37.84	75	38.37	38.03	103	40.54	40.34	126	39.37	40.00	150	39.25	39.67
29	33.76	33.47	53	37.53	37.57	81	43.43	43.11	104	39.98	40.56	127	40.04	38.96			
30	33.39	33.51	54	40.71	40.43	82	42.43	42.69	105	41.13	40.56	128	39.16	39.05			
31	33.43	33.33	55	40.50	40.43	83	42.76	42.47	106	40.54	40.47	129	38.87	39.10			
32	32.47	33.46	56	36.61	36.55	84	41.92	42.41	107	40.46	40.28	130	40.71	39.44			

Table 6 (Continued)

(K) Experimental and Estimated (Model 11) Heats of Evaporization for 69 Alkanes

no.	HV^0	HV^1	no.	HV^0	HV^1	no.	HV^0	HV^1	no.	HV^0	HV^1	no.	HV^0	HV^1	no.	HV^0	HV^1
6	26.42	27.16	18	34.24	33.73	30	37.86	37.73	43	44.75	44.63	55	44.81	44.80	67	43.95	43.91
7	24.59	25.12	19	32.88	32.94	31	37.93	37.69	44	44.75	44.71	56	41.91	41.93	68	41.00	40.95
8	21.78	21.98	20	33.02	32.61	32	39.02	38.81	45	42.28	42.19	57	40.57	40.67	69	41.00	41.05
9	31.55	31.88	21	35.22	34.86	33	39.40	39.80	46	43.79	43.65	58	40.17	40.33	70	38.10	38.30
10	29.86	29.92	22	32.04	31.61	34	36.91	36.83	47	42.87	42.96	59	42.23	42.27	71	41.75	41.82
11	30.27	29.98	23	41.48	41.50	35	35.13	35.51	48	42.87	42.78	60	42.93	42.92	72	42.02	42.08
12	27.69	27.28	24	39.68	39.59	36	37.22	37.09	49	42.82	42.60	61	41.42	41.95	73	42.55	42.59
13	29.12	28.73	25	39.83	39.73	37	37.61	37.75	50	42.66	42.71	62	40.84	41.01	74	42.93	42.93
14	36.55	36.66	26	39.67	39.77	38	38.52	38.77	51	43.84	43.84	63	42.28	42.38	75	43.36	43.34
15	34.80	34.74	27	37.29	37.25	39	37.99	37.96	52	42.98	43.05	64	43.84	43.80			
16	35.08	34.84	28	38.79	38.70	41	46.44	46.37	53	42.66	42.84	65	42.98	43.02			
17	32.43	32.30	29	37.76	37.96	42	44.65	44.48	54	44.81	44.74	66	43.04	43.11			

(L) Experimental and Estimated (Model 12) Heats of Atomization for 44 Alkanes

no.	HA^0	HA^1	no.	HA^0	HA^1	no.	HA^0	HA^1	no.	HA^0	HA^1	no.	HA^0	HA^1
3	4000.45	4080.53	12	7542.48	7500.16	21	8700.04	8687.15	30	9886.42	9902.99	39	9878.75	9857.12
4	5176.18	5220.79	13	7534.69	7500.86	22	8715.20	8659.99	31	9883.90	9875.92	40	9889.68	9848.89
5	5184.56	5200.84	14	8698.16	8692.15	23	9872.22	9866.84	32	9876.77	9875.12	41	11046.24	11048.55
6	6349.91	6368.40	15	8705.32	8699.83	24	9879.26	9882.51	33	9874.65	9874.11	68	11054.45	11067.42
7	6357.95	6355.55	16	8702.68	8695.09	25	9876.41	9880.83	34	9883.90	9865.64	69	11054.20	11103.13
8	6369.46	6332.77	17	8716.54	8691.57	26	9875.87	9881.90	35	9887.92	9918.30	70	11059.18	11170.47
9	7524.10	7525.61	18	8709.63	8683.19	27	9888.51	9889.62	36	9880.22	9854.99	71	11053.45	11068.42
10	7531.22	7523.42	19	8712.39	8711.98	28	9877.71	9879.87	37	9881.22	9882.30	75	11049.17	11046.56
11	7528.54	7517.61	20	8711.94	8674.90	29	9883.19	9902.84	38	9874.99	9872.99			

(M) Experimental and Estimated (Model 13) Heats of Formation for 54 Alkanes

no.	HF^0	HF^1	no.	HF^0	HF^1	no.	HF^0	HF^1	no.	HF^0	HF^1	no.	HF^0	HF^1	no.	HF^0	HF^1
4	126.23	129.95	13	177.90	177.06	22	204.99	200.90	31	218.34	219.46	40	226.05	222.42	62	240.62	244.46
5	134.61	140.12	14	187.95	188.27	23	208.59	208.90	32	211.68	211.08	41	228.35	229.90	63	236.22	236.20
6	146.54	148.62	15	195.10	195.07	24	215.62	215.59	33	209.38	208.62	44	235.26	233.77	68	238.94	240.29
7	154.58	155.48	16	192.43	191.58	25	212.77	212.33	34	220.27	218.68	45	246.31	244.39	69	237.85	239.11
8	168.60	166.63	17	206.37	202.75	26	212.23	212.54	35	224.29	227.15	56	241.58	240.24	70	243.50	252.61
9	167.30	168.12	18	195.31	193.66	27	223.99	223.50	36	216.58	217.61	57	243.34	245.01	71	237.31	236.31
10	174.42	174.97	19	202.22	200.39	28	214.53	214.57	37	217.59	215.11	58	253.43	249.15	72	231.82	236.88
11	171.74	171.27	20	201.68	197.98	29	216.04	217.60	38	210.39	210.68	59	239.95	239.69	74	228.10	232.96
12	185.68	182.09	21	189.83	187.49	30	220.14	221.44	39	215.12	214.30	61	242.71	240.01	75	233.67	231.05

(N) Experimental and Estimated (Model 14) Heats of Formation in Liquid for 62 Alkanes

no.	HFL^0	HFL^1	no.	HFL^0	HFL^1	no.	HFL^0	HFL^1	no.	HFL^0	HFL^1	no.	HFL^0	HFL^1	no.	HFL^0	HFL^1
2	22.50	22.51	13	49.48	49.12	24	60.98	61.16	35	61.97	63.02	58	70.11	69.47	75	65.85	65.03
3	28.79	30.14	14	53.63	53.82	25	60.34	60.37	36	60.63	60.65	59	67.18	67.00	76	71.95	72.37
4	35.34	35.99	15	54.93	55.04	26	60.17	60.36	37	60.98	60.39	61	67.88	67.59	77	74.04	73.58
5	36.95	37.90	16	54.35	54.22	27	62.63	62.27	38	59.69	59.57	62	66.97	68.28	80	73.58	72.89
6	41.40	41.83	17	57.05	56.07	28	60.40	60.50	39	60.46	60.01	63	66.33	66.18	108	72.84	73.87
7	42.95	43.04	18	54.83	54.35	29	61.47	61.34	40	62.40	61.22	68	66.54	66.55	121	72.53	73.04
8	45.61	44.88	19	56.17	56.00	30	62.26	62.26	41	65.64	66.13	69	66.40	66.91	126	77.32	76.61
9	47.52	47.78	20	56.07	54.98	31	61.58	61.22	44	66.82	66.59	70	66.95	69.89			
10	48.82	48.98	21	53.77	53.30	32	60.23	59.68	45	68.88	68.49	71	66.46	66.18			
11	48.28	48.18	22	56.63	55.51	33	59.88	59.45	56	67.57	67.23	72	65.18	66.36			
12	51.00	49.94	23	59.74	59.95	34	61.44	60.94	57	67.60	68.51	74	64.47	65.70			

(O) Experimental and Estimated (Model 15) Heats of Formation in Gas for 63 Alkanes

no.	HFG^0	HFG^1	no.	HFG^0	HFG^1	no.	HFG^0	HFG^1	no.	HFG^0	HFG^1	no.	HFG^0	HFG^1	no.	HFG^0	HFG^1
1	17.89	17.94	12	44.35	43.38	23	49.82	50.02	34	52.61	52.19	57	58.12	58.95	74	54.48	55.81
2	20.24	20.12	13	42.49	42.43	24	51.50	51.74	35	53.57	54.68	58	60.53	59.96	75	55.81	55.12
3	24.82	25.66	14	44.89	45.03	25	50.82	50.94	36	51.73	51.93	59	57.31	56.96	76	59.67	60.12
4	30.15	30.43	15	46.60	46.75	26	50.69	50.88	37	51.97	51.74	61	59.97	57.91	77	62.17	61.85
5	32.15	33.00	16	45.96	45.95	27	53.71	53.30	38	50.48	50.55	62	57.47	58.71	80	61.80	61.02
6	35.00	35.23	17	49.29	48.28	28	51.16	51.40	39	51.38	51.18	63	56.42	56.16	108	62.22	63.04
7	36.92	37.03	18	46.65	46.48	29	52.44	52.46	40	53.99	53.12	68	57.07	57.13	121	62.08	62.26
8	40.27	39.50	19	48.30	48.29	30	53.21	53.40	41	54.54	55.05	69	56.81	57.40	126	67.29	66.53
9	39.96	40.09	20	48.17	47.27	31	52.61	52.25	44	56.19	55.93	70	58.16	61.03			
10	41.66	41.83	21	45.34	45.14	32	50.91	50.60	45	58.83	58.37	71	56.67	56.45			
11	41.02	41.08	22	48.96	48.04	33	50.40	50.09	56	57.70	57.21	72	55.37	56.37			

1.03) for the ST (dyn/cm); no. 68 (MV_{exp} = 169.495, ΔMV = −9.557) for the MV (cm^3/mol); no. 71 (HC_{exp} = 219.50, ΔHC = −12.09), no. 146 (HC_{exp} = 223.70, ΔHC = 15.03), and no. 149 (HC_{exp} = 224.80, ΔHC = 15.58) for the HC ($J.K^{-1}\cdot mol^{-1}$); no. 70 (HF_{exp} = 243.50, ΔHF = 14.93) for the HF (kJ/mol); no. 3 (HFL_{exp} = 28.79, ΔHFL = 1.90) and

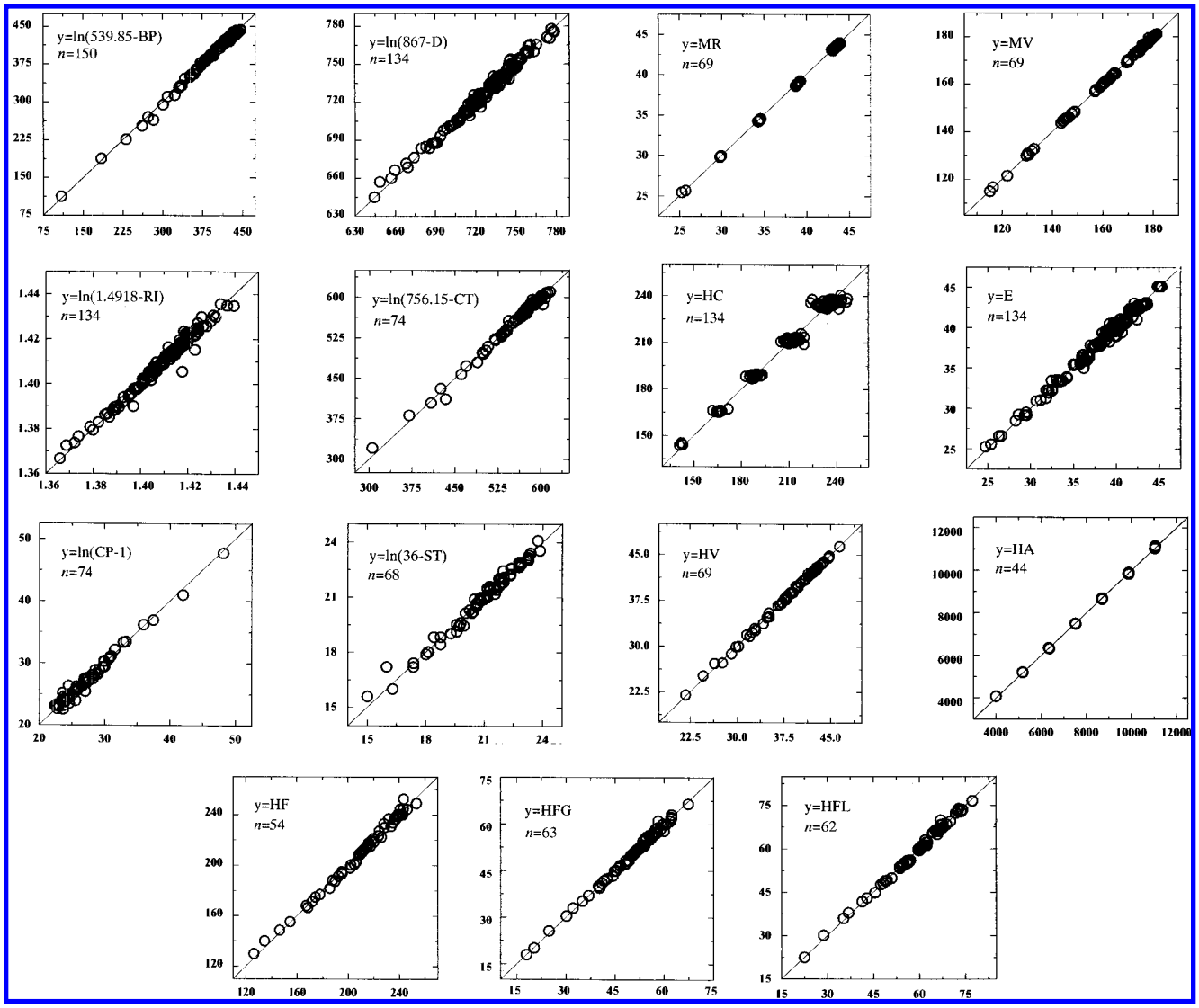

Figure 3. Plot of the property (y) estimated by model vs that observed experimentally for 15 properties of alkanes.

no. 70 (HFL_{exp} = 66.95, ΔHFL = 3.94) for the HFL (kJ/mol); no. 1 (HFG_{exp} = 17.89, ΔHFG = 6.81) and no. 70 (HFG_{exp} = 58.16, ΔHFG = 3.52) for the HFG (kJ/mol); no. 1 (BP_{exp} = 109.15, ΔBP = 145.02); no. 2 (BP_{exp} = 184.55, ΔBP = 9.68) and no. 8 (BP_{exp} = 282.65, ΔBP = −20.85) for the logarithmic models of BP (K); no. 2 (CT_{exp} = 305.42, ΔCT = 72.16), no. 8 (CT_{exp} = 433.75, ΔCT = −33.45), and no. 40 (CT_{exp} = 543.95, ΔCT = 25.08) for the logarithmic models of CT (K); no. 49 (CP_{exp} = 23.70, ΔCP = −1.28), no. 65 (CP_{exp} = 25.56, ΔCP = −1.79), no. 67 (CP_{exp} = 23.59, ΔCP = 1.88), no. 68 (CP_{exp} = 27.04, ΔCP = −3.26), and no. 70 (CP_{exp} = 24.58, ΔCP = −1.56) for the logarithmic models of CP (atm); no. 6 (ST_{exp} = 16.00, ΔST = 1.47), no. 7 (ST_{exp} = 15.00, ΔST = 0.76), and no. 68 (ST_{exp} = 23.38, ΔST = 1.22) for the logarithmic models of ST (dyn/cm). It has been found that there are six results with relative errors greater than 20%, and these are no. 1 (−88.30%) and no. 2 (21.54%) of the BP model, no. 2 (22.63%) of the CT model, no. 1 (38.07%) of the HFG model, no. 1 (132.86%) of the logarithmic BP model, and no. 2 (23.63%) of the logarithmic CT model.

The 15 models, model 16, 17, 18, 19, 20, 21, 7, 8, 9, 10, 11, 12, 13, 14, and 15, are then utilized to estimate the physical properties or thermodynamic functions of alkanes; the estimated results are listed in Table 6. To intuitively express the relationship of property to the MEDV, the properties (y_{EST}) estimated by QSPR models being plotted vs the properties (y_{OBS}) observed experimentally are shown in Figure 3.

Comparison of the Results. As for the λ vector,[28,31] the molecular electronegative distance vector is only utilized to construct the QSPR model between the MEDV and physical properties or thermodynamic functions of alkanes, not to select and optimize various structural parameters from a large database containing many descriptors. The results using the MEDV methodology are on average better than the results using the λ vector method. The estimated rms of boiling point for 150 alkanes by a logarithm model in the ref 28 is rms = 4.985 °C and correlation coefficient R = 0.9948, while rms = 3.22 °C and R = 0.9978 in the present paper. In the literature,[31] the estimated rms values of HC, E, HV, HA, HF, HFL, and HFG for alkanes are respectively 4.04, 0.53, 0.39, 51.56, 2.22, 0.79, and 0.73, and the estimated R is 0.9881, 0.9930, 0.9977, 0.9996, 0.9976, 0.9977, and 0.9977. In our present paper, rms is 3.81, 0.48, 0.22, 29.98, 2.58, 0.72, and 0.70, and R is 0.9886, 0.9937, 0.9991, 0.9998,

0.9960, 0.9977, and 0.9975, respectively. Furthermore, the MEDV using an *add operations* is more simple than the λ vector using *multiply operations*.

In the same way, comparison between the MEDV and that from other literature is also performed. In ref 34 containing 150 alkanes (all C_1-C_{10}) together with boiling points, the structural descriptors were selected from 16 distance indices and two connective indices by means of an optimization method to construct five three-parameter QSPR equations of boiling points and seven four-parameter QSPR equations in which the lowest rms = 5.93 °C in the three-parameter QSPRs and 5.15 °C in four-parameter models. For the MV, MR, HV, CT, CP, ST, and so on,[36] the estimated rms values are 2.8, 0.05, 0.4, 5.4, 0.7, and 0.3, respectively, while in the present paper the rms values are 0.359, 0.0643, 0.22, 5.30, 0.58, and 0.26, respectively. For the boiling point, ref 2 gave a QSPR model of 245 alkanes and alcohols with $R = 0.97$ and rms = 7.98 K and ref 10 gave a high-quality QSPR model of 298 heterogeneous compounds with rms = 5.36 K. Reference 10 also gave a QSPR model of 165 heterogeneous compounds and critical temperatures with rms = 6.62 K.

CONCLUSION

Fifteen models have been developed to estimate and predict 15 physical properties or thermodynamic functions including BP, *D*, RI, CT, CP, ST, MR, MV, HC, *E*, HV, HA, HF, HFL, and HFG of alkanes with a high degree of accuracy. In general, these models have provided more accurate results than many previous methodologies in the literature. It is foreseeable that the MEDV vector would be utilized widely in QSPR/QSAR and/or other related studies. Further research is in progress.

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