Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C_nH_{2n+2} (n = 6 to 8)

Hideo Watanabe*

National Metrology Institute of Japan, AIST 1-4, Umezono 1-chome, Tsukuba, Ibaraki 305-8563, Japan

Experimental values of the thermal conductivity λ and thermal diffusivity κ of sixteen pure branched alkanes (C_nH_{2n+2}; n = 6 to 8) are presented in the temperature range −15 °C to 70 °C under atmospheric or saturation pressure. Measurements were made with the transient hot-wire method, and in the analysis, the temperatures T_λ and T_κ (associated with both λ and κ) were used. The thermal diffusivity values are corrected by the factors k_f (=1.0076 to 0.9892), which are determined by reference to the heat capacity (at 298.15 K) of heptane as a reference material, for data sets obtained with different configurations of the experiments. Heat capacities [volumic, $c_p\rho$; specific, c_p; and molar, $C_{m,p}$] are derived from the relationship $c_p\rho = \lambda/\kappa$, with values for the density and the molar mass. The relevance of these thermal properties to the boiling point, density, molar density, and velocity-of-sound is examined, together with the results of normal alkanes (n = 6 to 8) and isopentane. The uncertainty of the data is estimated to be 0.4% for the thermal conductivity (absolutely measured) and about 1.8% for the thermal diffusivity (with a coverage factor k_p = 2; p = 95%), although that of λ (not for κ) is possibly inferior for a few substances containing a little larger impurity (i.e. mainly other isomers).

Introduction

The thermophysical transport properties of alkanes, including their isomers, are important for investigating the mechanism of the conduction heat transfer or various chemical processes, but systematically obtained data are considered insufficient. A procedure was previously introduced for simultaneously measuring the thermal conductivity and thermal diffusivity with the transient hot-wire (THW) method, and the results for n-alkanes C_nH_{2n+2} (n = 5 to 10) and methylbutane (isopentane) are reported in the temperatures range −20 °C to 70 °C under atmospheric pressure.[1−3] The summarized results of the measurements of sixteen kinds of branched alkanes, under the same conditions, were reported as follows: C_6H_{14} (2,2-dimethylbutane, 2,3-dimethylbutane, 2-methylpentane, 3-methylpentane), C_7H_{16} (2,2,3-trimethylbutane, 2,2-dimethylpentane, 3,3-dimethylpentane, 2,4-dimethylpentane, 2,3-dimethylpentane, 2-methylhexane, 3-methylhexane, 3-ethylpentane), and C_8H_{18} (2,2,4-trimethylpentane [isooctane], 2,3,4-trimethylpentane, 2-methylheptane, 3-methylheptane).[4−6] The present paper illustrates and provides the tabular data, examining the relevance of the thermal properties to the boiling point, density (or molar density), and velocity-of-sound.

The results for the thermal conductivity and thermal diffusivity were analyzed using two temperatures, T_λ and T_κ, which refer to each measured value.[2] As stated before,[2] the small diameter of the wire (platinum, ≈15 μm) was determined by the mass and the density of the piece of wire to directly obtain the thermal diffusivity, though the thermal diffusivity values were substantially corrected by factors k_f (=1.0076 to 0.9892). This correction is equivalent to adjustment for the radius of the wires.

The effect of the radiation heat transfer (by photons) is regarded as a part of ordinary heat conduction phenomena by carriers such as phonons, electrons, and molecules.[2]

* To whom correspondence should be addressed. Phone: +81-298-61-4395. Fax: +81-298-61-4039. E-mail: watanabe-hideo@aist.go.jp.

Measurement Procedure

THW Model. To summarize the system,[1,2] an actual model of the THW method (Figure 1) is described by a transfer function having a feedback loop [i.e., the heating rate of the wire, $q(t) = Q_0(1 + A\Delta T(t) + B\Delta T^2(t)(t) + ...)$, $t \geq 0$], where A and B are fixed by the temperature dependence of the wire resistance and the circuit arrangement, including the type of power supply. The temperature rise of the wire $\Delta T(t)$ [inverse-Laplace transformation of $\Theta(s)$] (if λ and κ are not dependent on the temperature) is as follows:[2,3]

$$\Delta T(t) = \left(\frac{Q_0}{4\pi\lambda}\right)\left\{\ln\frac{4\kappa t}{a^2\mathrm{C}} + \frac{a^2}{2\kappa t}\left(\frac{k-1}{k}\ln\frac{4\kappa t}{a^2\mathrm{C}} + 1\right) - \frac{a^2}{4\kappa_W t} + \frac{\lambda}{2\lambda_W} - \left(\frac{a^2}{4\kappa t}\right)^2\left[3\left(1-\frac{1}{k}\right)^2\left(\ln\frac{4\kappa t}{a^2\mathrm{C}}\right)^2 + \left(1+\frac{4}{k}-\frac{6}{k^2}\right)\left(\ln\frac{4\kappa t}{a^2\mathrm{C}}\right) - \left(\frac{\pi^2}{2}+\frac{3}{2}\right) + \frac{\pi^2+4}{k} - \frac{\pi^2}{2k^2}\right] + ...\right\} + A\left(\frac{Q_0}{4\pi\lambda}\right)^2\left\{\left(\ln\frac{4\kappa t}{a^2\mathrm{C}}\right)^2 + \frac{a^2}{\kappa t}\left(\ln\frac{4\kappa t}{a^2\mathrm{C}} + 1\right) - \frac{\pi^2}{6} + ...\right\} + A^2\left(\frac{Q_0}{4\pi\lambda}\right)^3\left\{\left(\ln\frac{4\kappa t}{a^2\mathrm{C}}\right)^3 - \frac{\pi^2}{2}\ln\frac{4\kappa t}{a^2C} + 2\zeta(3) + ...\right\} + B\left(\frac{Q_0}{4\pi\lambda}\right)^3\left\{\left(\ln\frac{4\kappa t}{a^2\mathrm{C}}\right)^3 - \frac{\pi^2}{3}\ln\frac{4\kappa t}{a^2\mathrm{C}} + 2\zeta(3) + ...\right\} \quad (1)$$

where λ and κ are the thermal conductivity and thermal diffusivity of the sample and λ_W and κ_W are those of the wire material (platinum), a is the radius of the hot-wire (≈7.5 μm), k is the ratio of volumic heat capacities (at constant pressure) of the sample and wire materials [$c_p\rho/(c_p\rho)_W$], C is the mathematical constant (=e^γ; γ, Euler's constant), and $\zeta(3)$ is the zeta function of n = 3 and so forth.[2]

10.1021/je020125e CCC: $25.00
Published on Web 11/02/2002

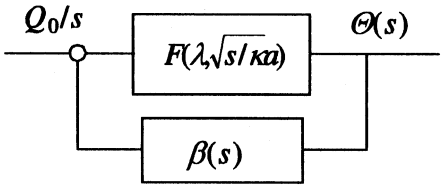

Figure 1. Equivalent diagram for the transient hot-wire method with a feedback loop. $F(\lambda, (s/\kappa)^{1/2}a)$ is the ideal transfer function involving both λ and κ as parameters, $\beta(s)$ is a feedback transfer function, Q_0/s is the step input of heat generation in the wire, and $\Theta(s)$ is the corresponding temperature rise.

Effective Temperature T_λ and T_κ to be Referred to λ and κ. When the temperature dependence of the thermal conductivity of the sample is χ and that of the volumic heat capacity is ϕ,

$$\lambda = \lambda_0(1 + \chi\Delta T) \tag{2}$$

$$c_p\rho = (c_p\rho)_0(1 + \phi\Delta T) \tag{3}$$

$$\kappa = \lambda/(c_p\rho) = \kappa_0\{1 + (\chi - \phi)\Delta T\} \tag{4}$$

where λ_0, $(c_p\rho)_0$, and κ_0 are the properties at $T = T_0$.

Then T_λ and T_κ are derived as follows:[2]

$$T_\lambda = T_0 + \Delta T_\lambda = T_0 + \{1 + (\phi/\chi)\}\Delta T_m - (\chi - \phi)(Q_0/4\pi\lambda_0)^2 \ln 4 \tag{5}$$

and

$$T_\kappa = T_0 + \Delta T_\kappa = T_0 + \{(\phi + \chi)/(\chi - \phi)\} \times \{\Delta T_m \ln(4\kappa_0 s/a^2 C) - (1/2)(Q_0/4\pi\lambda_0)[(\ln 4\kappa_0 s/a^2 C)^2 - (\ln t_f/s)(\ln t_i/s)]\} + (Q_0/4\pi\lambda_0)\ln 4 \tag{6a}$$

or, as another equivalent expression,

$$T_\kappa = T_0 + \Delta T_\kappa = T_0 + \{(\phi + \chi)/(\chi - \phi)\} \times \{(1/2)(Q_0/4\pi\lambda_0)^{-1}\Delta T_m{}^2 - (1/8)(Q_0/4\pi\lambda_0)(\ln t_f/t_i)\} + (Q_0/4\pi\lambda_0)\ln 4 \tag{6b}$$

where

$$\Delta T_m = (1/2)\{\Delta T(t_i) + \Delta T(t_f)\} \tag{7}$$

and t_i and t_f are the elapsed times assigned to the initial and final acquisition data for each experiment.

The temperature T_λ is different by the small factor $(\phi/\chi)\Delta T_m - (\chi - \phi)(Q_0/4\pi\lambda_0)^2 \ln 4$ from the temperature $T_m = T_0 + \Delta T_m$. The magnitude of the heat capacity coefficient, ϕ, for an ordinary hydrocarbon is probably small in comparison with the χ for thermal conductivity. Therefore, the substitution of (commonly used) T_m, which has so far been assigned to the measured value λ, for the temperature T_λ is not such a serious problem. However, the use of the temperature $T_\kappa = T_0 + \Delta T_\kappa$ in place of (commonly used) T_0 is more significant.

Practical Measurement System. The experimental system and procedure are the same as those reported previously[2,3] with two hot-wire sensors (4-terminal resistance, i.e., AC and BD cells). The data sampling was carried out in the same way as in previous experiments. The sampling interval was 50 ms, the integrating time was always 20 ms, and the number of data was usually 20. The elapsed times, t_i and t_f, were nominally $t_i \approx 0.03$ s and $t_f \approx 1$ s in the present case. The set of data $\{\Delta T(t_j), t_j\}$ was fitted to eq 1.

Table 1. Empirical Correction Factors for the Thermal Diffusivity Data

	set A	set B	set C	set D
k_f	1.005 61	0.989 17	1.007 65	0.991 81

For the practical experiment, the temperature rise $\Delta T(t_f)$ (maximum value) is mostly about 1.5 to 2.5 K (or 3 K in case especially large). As long as the temperature of the fluid material does not traverse a proper phase transition temperature (this means the equilibrium state), the material is considered not to partially transform its phase for the duration of heating the wire (although the material is not in the equilibrium state), even if at a very short time smaller than $t_i = 0.03$ s. The materials used in the present study are considered not to make a phase transition in the range of temperature of the present study.

Correction Factors k_f for Thermal Diffusivity. The data for a regular configuration are designated set A for cell AC, and those for an inverted position, set C: similarly, the regular position for cell BD is associated with set B and the inverted position is for set D. To eliminate the systematic differences resulting from the cells and the configuration of each experiment, the data for thermal diffusivity were adjusted by the correction factor k_f, which is based on the values of *n*-heptane: $c_p = 2.2429$ kJ·kg^{-1}·K^{-1} and $\rho = 679.46$ kg/m^3 at 298.15 K,[7] and the relationship $\kappa = \lambda/c_p\rho$ (where $\lambda_{298.15\ K}$ was determined from the results by an experiment carried out separately for calibration). Then the correction factors k_f for thermal diffusivity were introduced as shown in Table 1. Measured thermal diffusivity data are multiplied by k_f for the respective configuration. These adjustments are about +0.7% for cell AC and −1.0% for cell BD. This corresponds to the practical adjustment for the diameter ($\approx$15 μm) of the wire by about +0.35% for cell AC and −0.5% for cell BD, complying with the systematic difference due to unknown factors when the cells are inverted, such as for configurations A and C for cell AC or B and D for cell BD.

Results

Materials. The liquid samples employed in the present measurements were obtained from various chemical product suppliers. We used them without any purification and removing dissolved water or air, by reason that they are mostly costly materials. The transfer of sample to the hot-wire glass-tube[2] was made with syringe and siphon, after roughly exhausting inside, so as to keep it as far away as possible from long exposure to the atmosphere.

The reagents C_6H_{14} were supplied by Wako Pure Chemical Industries Ltd., Japan. The purities stated by the supplier were as follows: 2-methylpentane, 99% with residuals 0.01%; 3-methylpentane, 98% with residuals 0.01%; 2,2-dimethylbutane, 97% with residuals 0.01%; 2,3-dimethylbutane, 98% with residuals 0.01%. The purities of the reagents C_7H_{16}were as follows: 2-methylhexane, 98% (Wako Pure Chemical Industries, Ltd., Lot No. ACG7389); 3-methylhexane, 99% (Wako Pure Chemical Industries, Ltd., Lot No. KSL23062000); 2,2-dimethylpentane, 99% (Wako Pure Chemical Industries, Ltd., Lot No. ACQ2765); 2,3-dimethylpentane, 98% with residual 0.01% (Wako Pure Chemical Industries, Ltd., Lot No. KSL3011); 2,4-dimethylpentane, 97% (Tokyo Chemical Industries, Ltd., Lot No. AV01); 3,3-dimethylpentane, 98% (Wako Pure Chemical

Table 2. Coefficients of Eqs 8 and 9[a]

material	cell	N (data)	λ_0/W·m^{-1}·K^{-1}	$A/10^{-4}$	$\kappa_0/10^{-8}$ m^2·s^{-1}	$B/10^{-2}$
2,2-dimethylbutane	AC,BD	60	0.100 63(3)	−2.909(12)	7.142(06)	−2.433(21)
2,3-dimethylbutane	AC,BD	60	0.107 61(6)	−2.924(16)	7.456(10)	−2.299(27)
2-methylpentane	AC,BD	60	0.112 72(5)	−3.103(14)	7.787(09)	−2.507(25)
3-methylpentane	AC,BD	60	0.114 16(5)	−3.105(14)	7.870(09)	−2.484(27)
2,2,3-trimethylbutane	AC	30	0.101 05(4)	−2.435(13)	6.921(14)	−2.143(39)
2,2-dimethylpentane	AC	30	0.104 61(5)	−2.658(14)	7.193(12)	−2.450(32)
3,3-dimethylpentane	AC	32	0.106 76(4)	−2.671(12)	7.317(15)	−2.600(41)
2,4-dimethylpentane	BD	30	0.108 91(5)	−2.767(14)	7.461(14)	−2.393(37)
2,3-dimethylpentane	AC	48	0.112 74(6)	−2.739(14)	7.737(18)	−2.718(43)
2-methylhexane	BD	30	0.117 71(4)	−2.885(11)	8.014(10)	−2.214(27)
3-methylhexane	BD	53	0.118 39(5)	−2.873(12)	8.108(12)	−2.399(27)
3-ethylpentane	BD	30	0.120 34(5)	−3.000(13)	7.905(11)	−2.270(30)
2,2,4-trimethylpentane	AC	30	0.100 71(3)	−2.378(09)	6.998(12)	−2.192(37)
2,3,4-trimethylpentane	BD	30	0.109 31(3)	−2.333(08)	7.045(08)	−1.981(24)
2-methylheptane	BD	30	0.120 58(2)	−2.681(07)	7.946((08)	−2.089(23)
3-methylheptane	AC	30	0.121 62(2)	−2.696(05)	7.989(10)	−2.179(27)

[a] The numbers in parentheses following the coefficients are the numerical values of the standard uncertainties referred to in the corresponding last digits.

Table 3. Experimental Data for 2,2-Dimethylbutane: Means of Four (A, B, C, and D) Results[a]

ϑ_0/°C	p_0/MPa	ϑ_λ/°C	λ/W·m^{-1}·K^{-1}	ϑ_κ/°C	$\kappa/10^{-8}$ m^2·s^{-1}	$(Q_0/4\pi\lambda)$/K
23.8438	0.1013	24.8334	0.093 21	26.1567	6.480	0.2047
23.8450	0.1013	25.2658	0.093 07	27.1640	6.458	0.2944
23.8444	0.1013	25.7551	0.092 89	28.2937	6.411	0.3994
5.7734	0.1013	6.7120	0.098 54	8.0172	6.939	0.1883
5.7734	0.1013	7.0865	0.098 42	8.9112	6.916	0.2641
5.7731	0.1013	7.5832	0.098 22	10.0787	6.853	0.3682
−16.5354	0.1013	−15.6704	0.105 46	−14.4096	7.540	0.1675
−16.5352	0.1013	−15.3102	0.105 28	−13.5331	7.493	0.2387
−16.5352	0.1013	−14.8541	0.105 11	−12.4189	7.458	0.3288
−2.5855	0.1013	−1.6622	0.101 12	−0.3568	7.156	0.1829
−2.5857	0.1013	−1.3057	0.101 00	0.5040	7.135	0.2541
−2.5848	0.1013	−0.8337	0.100 80	1.6262	7.077	0.3508
45.1369	0.1013	46.1985	0.087 45	47.5682	6.029	0.2251
45.1370	0.1013	46.5972	0.087 29	48.4722	5.992	0.3119
45.1376	0.1013	47.1307	0.087 09	49.6767	5.949	0.4290

[a] Thermal diffusivity values were adjusted by factors k_f.

Table 4. Experimental Data for 2,3-Dimethylbutane: Means of Four (A, B, C, and D) Results[a]

ϑ_0/°C	p_0/MPa	ϑ_λ/°C	λ/W·m^{-1}·K^{-1}	ϑ_κ/°C	$\kappa/10^{-8}$ m^2·s^{-1}	$(Q_0/4\pi\lambda)$/K
23.4063	0.1013	24.4766	0.100 04	25.7997	6.799	0.1908
23.4062	0.1013	24.9065	0.099 90	26.7476	6.771	0.2678
23.4058	0.1013	25.4510	0.099 72	27.9360	6.736	0.3654
3.8215	0.1013	4.8300	0.106 06	6.1403	7.305	0.1751
3.8213	0.1013	5.2255	0.105 91	7.0415	7.270	0.2448
3.8214	0.1013	5.7592	0.105 73	8.2424	7.234	0.3379
−17.2699	0.1013	−16.3387	0.112 78	−15.0574	7.873	0.1581
−17.2700	0.1013	−15.9610	0.112 66	−14.1687	7.845	0.2225
−17.2702	0.1013	−15.4611	0.112 46	−13.0176	7.787	0.3084
43.6796	0.1013	44.9555	0.094 29	46.4780	6.385	0.2302
43.6795	0.1013	45.2964	0.094 16	47.2111	6.346	0.2937
43.6798	0.1013	45.9111	0.093 98	48.5239	6.309	0.4059
61.7921	0.1013	63.1358	0.089 57	64.6953	6.041	0.2459
61.7927	0.1013	63.5020	0.089 44	65.4668	6.009	0.3141
61.7925	0.1013	64.1453	0.089 25	66.8127	5.967	0.4336

[a] Thermal diffusivity values were adjusted by factors k_f.

Industries, Ltd., Lot No. ELJ4043); 2,2,3-trimethylbutane, 99% (Aldrich Chemical Co., Lot No. 14308PU); 3-ethylpentane, 93% (Tokyo Chemical Industries, Ltd., Lot No. E046).The purities of the reagents C_8H_{18} were as follows: 2-methylheptane, 99% (Aldrich Chemical, Lot No. CI-03022B1); 3-methylheptane, 95% (Lancaster Co., Lot No. 00003331); 2,2,4-trimethylpentane, 99% (Dojin-Do Laboratories, Japan, Lot No. ZA263); 2,3,4-trimethylpentane, 99% (Aldrich Chemical, Lot No. JR-2516AQ).

Experimental Data. The experiments for the 16 isomers of alkanes (nearly atmospheric liquid), C_nH_{2n+2} (n = 6 to 8), were carried out at three heating rates Q_0 at a bath temperature T_0 for respective cell settings. The measured data were fitted in terms of the following formulas:

$$\lambda/\mathrm{W\cdot m^{-1}\cdot K^{-1}} = \lambda_0/\mathrm{W\cdot m^{-1}\cdot K^{-1}} - A/(T/\mathrm{K} - 273.15) \quad (8)$$

and

$$\kappa/10^{-8}\,\mathrm{m^2\cdot s^{-1}} = \kappa_0/10^{-8}\,\mathrm{m^2\cdot s^{-1}} - B/(T/\mathrm{K} - 273.15) \quad (9)$$

The values of the coefficients of eqs 8 and 9 are shown in Table 2, where the numbers in parentheses following the

Table 5. Experimental Data for 2-Methylpentane: Means of Four (A, B, C, and D) Results[a]

ϑ_0/°C	p_0/MPa	ϑ_λ/°C	λ/W·m^{-1}·K^{-1}	ϑ_κ/°C	$\kappa/10^{-8}$ m^2·s^{-1}	$(Q_0/4\pi\lambda)$/K
23.2813	0.1013	24.2069	0.104 92	25.5142	7.113	0.1865
23.2813	0.1013	24.5557	0.104 79	26.3534	7.091	0.2575
23.2811	0.1013	25.0067	0.104 59	27.4249	7.038	0.3517
−17.3835	0.1013	−16.5853	0.118 19	−15.3637	8.232	0.1511
−17.3837	0.1013	−16.2633	0.118 05	−14.5583	8.181	0.2135
−17.3838	0.1013	−15.8572	0.117 89	−13.5352	8.152	0.2918
2.9977	0.1013	3.8602	0.111 40	5.1279	7.654	0.1684
2.9961	0.1013	4.1952	0.111 25	5.9485	7.608	0.2358
2.9976	0.1013	4.6518	0.111 07	7.0658	7.572	0.3267
40.0190	0.1013	41.0025	0.099 89	42.3496	6.711	0.2028
40.0190	0.1013	41.3576	0.099 78	43.1891	6.694	0.2767
40.0188	0.1013	41.8387	0.099 59	44.3166	6.651	0.3788
54.0924	0.1013	55.1427	0.095 97	56.5527	6.423	0.2196
54.0925	0.1013	55.4897	0.095 83	57.3584	6.394	0.2935
54.0931	0.1013	56.0029	0.095 64	58.5477	6.356	0.4037

[a] Thermal diffusivity values were adjusted by factors k_f.

Table 6. Experimental Data for 3-Methylpentane: Means of Four (A, B, C, and D) Results[a]

ϑ_0/°C	p_0/MPa	ϑ_λ/°C	λ/W·m^{-1}·K^{-1}	ϑ_κ/°C	$\kappa/10^{-8}$ m^2·s^{-1}	$(Q_0/4\pi\lambda)$/K
−17.2667	0.1013	−16.4673	0.119 63	−15.2642	8.314	0.1495
−17.2671	0.1013	−16.1513	0.119 48	−14.4799	8.269	0.2099
−17.2671	0.1013	−15.7159	0.119 29	−13.4006	8.220	0.2936
2.6718	0.1013	3.5559	0.112 93	4.8344	7.743	0.1705
2.6720	0.1013	3.8693	0.112 79	5.5936	7.705	0.2321
2.6725	0.1013	4.3138	0.112 59	6.6714	7.666	0.3196
22.2974	0.1013	23.2375	0.106 60	24.5415	7.208	0.1871
22.2969	0.1013	23.5938	0.106 51	25.3952	7.198	0.2582
22.2969	0.1013	24.0504	0.106 34	26.4791	7.162	0.3508
40.0714	0.1013	41.0712	0.101 32	42.4192	6.804	0.2030
40.0714	0.1013	41.4420	0.101 21	43.2932	6.796	0.2782
40.0715	0.1013	41.9327	0.101 01	44.4301	6.746	0.3809
54.1673	0.1013	55.2051	0.097 36	56.5755	6.508	0.2138
54.1694	0.1013	55.5989	0.097 23	57.4862	6.494	0.2948
54.1695	0.1013	56.1149	0.097 05	58.6659	6.444	0.4048

[a] Thermal diffusivity values were adjusted by factors k_f.

Table 7. Experimental Data for 2,2,3-Trimethylbutane: Means of the A and C Results[a]

ϑ_0/°C	p_0/MPa	ϑ_λ/°C	λ/W·m^{-1}·K^{-1}	ϑ_κ/°C	$\kappa/10^{-8}$ m^2·s^{-1}	$(Q_0/4\pi\lambda)$/K
22.5001	0.1013	23.1437	0.095 16	24.0520	6.293	0.1601
22.4989	0.1013	23.4332	0.095 08	24.7617	6.323	0.2296
22.4987	0.1013	23.7232	0.094 97	25.4620	6.305	0.3019
−16.4985	0.1013	−15.8823	0.105 11	−14.9358	7.279	0.1373
−16.4997	0.1013	−15.6193	0.104 99	−14.2668	7.269	0.1962
−16.4949	0.1013	−15.3425	0.104 86	−13.5705	7.260	0.2567
3.8248	0.1013	4.4654	0.100 05	5.4151	6.809	0.1489
3.8256	0.1013	4.7463	0.099 90	6.1108	6.795	0.2143
3.8256	0.1013	5.0197	0.099 80	6.7829	6.765	0.2796
40.0829	0.1013	40.7611	0.091 08	41.7034	6.001	0.1714
40.0824	0.1013	41.0580	0.090 98	42.4158	6.002	0.2459
40.0830	0.1013	41.3664	0.090 85	43.1503	5.985	0.3243
57.3163	0.1013	58.0262	0.087 18	58.9964	5.721	0.1825
57.3166	0.1013	58.3327	0.087 06	59.7194	5.705	0.2619
57.3165	0.1013	58.6412	0.086 90	60.4376	5.663	0.3456

[a] Thermal diffusivity values were adjusted by factors k_f.

coefficients are the numerical values of the standard uncertainties referred to in the corresponding last digits of the quoted results for the intercept and slope. The data used in fitting are summarized in Tables 3−18 (in which the temperature is ϑ/°C = T/K − 273.15), as the mean of four results (sets A, B, C, and D) or two results (sets A and C with cell AC, or sets B an D with cell BD) obtained experimentally with an equivalent heating rate of Q_0 to reduce the amount of data.

Figure 2 illustrates the respective correlation lines for the thermal conductivity and thermal diffusivity together with those of *n*-alkanes (C_nH_{2n+2}, n = 5 to 8) and isopentane.[2] The symbol (○) at the end of the line indicates the data extrapolated to the boiling point. Figures 3−5 show the deviations for 16 isomers of n = 6−8 of the measured values (together with the thermal conductivities of 2,3-dimethylpentane and 2-methylhexane[8]) from eqs 8 and 9.

Naturally, the specific (massic) heat capacity at constant pressure c_p can be derived from the thermal conductivity λ, the thermal diffusivity κ, and the density ρ using the equation $\kappa = \lambda/c_p\rho$. The density and molar mass of the sample were obtained from the literature.[9] Table 19 lists the values determined for the properties at a nominal temperature of 298.15 K together with the values of the molar heat capacity[7,9] (including results of *n*-alkanes obtained previously[3]). The various (volumic, $c_p\rho$; specific, c_p; and molar, $C_{m,p}$) heat capacities are in agreement with most of the values found in the literature.

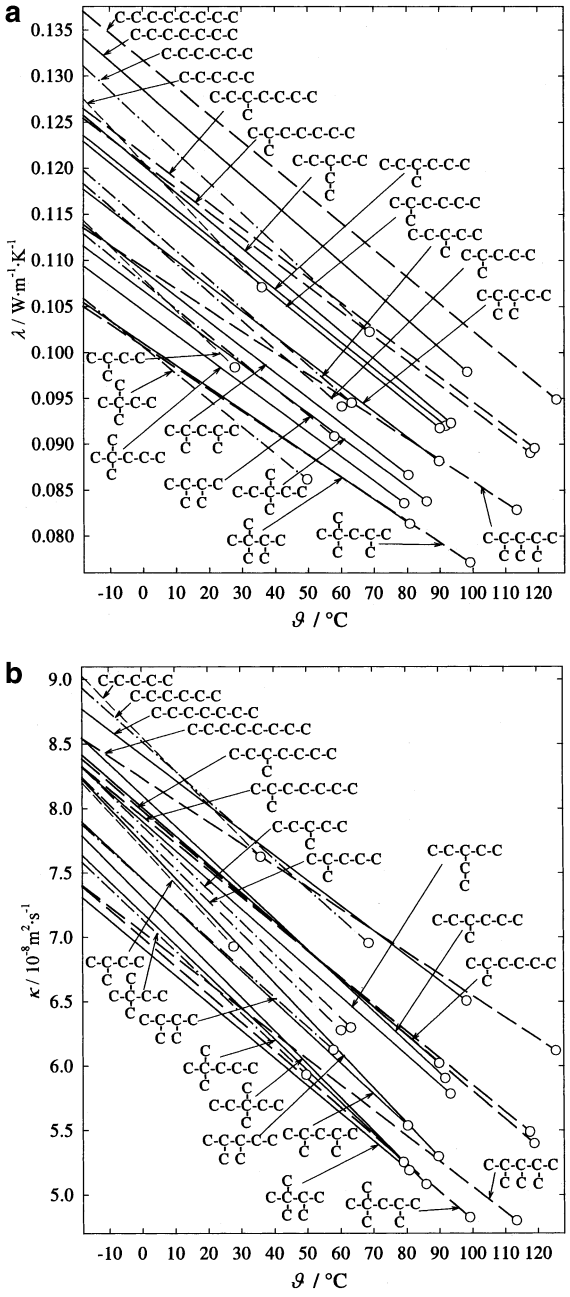

Figure 2. Fitting for alkanes C_nH_{2n+2} (n = 5 to 8) together with those of *n*-alkanes and isopentane:[3] (- - -), C_5H_{12}; (— · —), C_6H_{14}; (—), C_7H_{16} ; (— — —), C_8H_{18}. The mark (○) at the edge of the straight line expresses the values extrapolated at the boiling point: (a) thermal conductivity; (b) thermal diffusivity. Values were adjusted by factors k_f.

Relevance to Other Properties. The thermal transport properties are considered to naturally have relevance to the boiling point. Parts a, b, and c of Figure 6 indicate the thermal conductivity, thermal diffusivity, and molar heat capacity at 298.15 K versus the boiling point T_b, respectively. The values of thermal conductivity and thermal diffusivity systematically form the respective line corresponding to the number of carbons and the position or number of the methyl radical branching alkyl. The values of the molar heat capacity $C_{m,p}$ are almost constant for isomers having the same molar mass M. The volumic ($c_p\rho$) and specific (c_p) heat capacities also act similarly to $C_{m,p}$. Figure 7 shows these properties as a function of the density at 298.15 K.

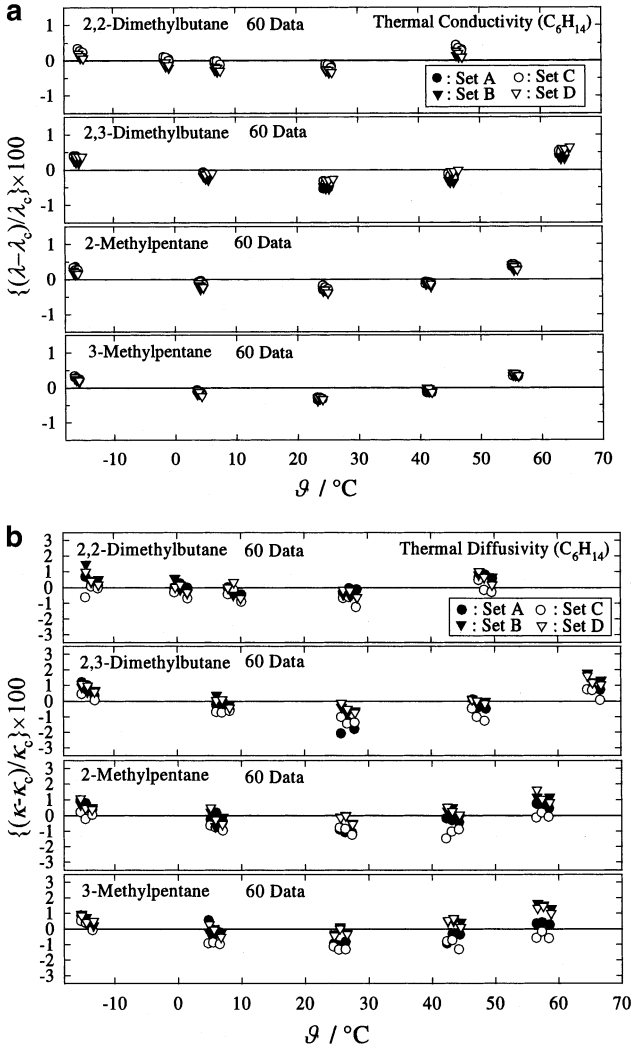

Figure 3. Deviations of measured values from the formulas (eqs 8 and 9 with coefficients listed in Table 2) respectively fitted for four isomers of C_6H_{14}: (a) thermal conductivity; (b) thermal diffusivity. Values were adjusted by factors k_f.

Prediction of thermal transport properties of pure organic liquids has been investigated, and an example of the original equations is given as follows:[10,11]

$$\kappa = \lambda/c_p\rho = A(\rho/M)^{1/3} \qquad (10)$$

where A is a parameter corresponding to the kind of substance and M is the molar mass of a pure substance (i.e. ρ/M means the molar density or M/ρ means the molar volume). However, the value A is variable, and the equation is modified considering the effects of the molecular configuration (including parameters such as the boiling temperature T_b, the molar latent heat of evaporation $\Delta_{vap}H$, the factor due to structure ϕ, etc.).[12]

Figure 8 expresses the value $A = \kappa/(\rho/M)^{1/3}$ at 298.15 K against T_b. The normal alkanes are in a straight line, and the value of toluene[3] as a reference is interestingly consistent with those of the normal alkanes though its molar density differs greatly from those of the alkanes. The isomers form a family of straight lines between carbon number groups having similarity in their isomer configurations. The correspondence between the predicted and measured properties (or the relations to the other thermal properties) will be discussed elsewhere.[13]

Table 8. Experimental Data for 2,2-Dimethylpentane: Means of the A and C Results[a]

ϑ_0/°C	p_0/MPa	ϑ_λ/°C	λ/W·m^{-1}·K^{-1}	ϑ_κ/°C	$\kappa/10^{-8}$ m^2·s^{-1}	$(Q_0/4\pi\lambda)$/K
22.5625	0.1013	23.1657	0.098 19	23.9952	6.566	0.1609
22.5633	0.1013	23.5406	0.098 03	24.8815	6.526	0.2631
22.5630	0.1013	23.8741	0.097 94	25.6708	6.492	0.3558
−17.5637	0.1013	−16.9946	0.109 38	−16.1416	7.663	0.1340
−17.5635	0.1013	−16.6334	0.109 15	−15.2527	7.582	0.2228
−17.5634	0.1013	−16.3108	0.109 03	−14.4538	7.558	0.3011
1.7077	0.1013	2.3031	0.104 13	3.1637	7.153	0.1475
1.7079	0.1013	2.6752	0.103 86	4.0575	7.062	0.2449
1.7072	0.1013	2.9826	0.103 70	4.7993	7.026	0.3253
43.4577	0.1013	44.0745	0.092 88	44.8983	6.096	0.1734
43.4589	0.1013	44.4754	0.092 64	45.8263	6.049	0.2894
43.4591	0.1013	44.7974	0.092 51	46.5730	6.025	0.3833
63.1278	0.1013	63.7572	0.087 93	64.5746	5.673	0.1865
63.1281	0.1013	64.1557	0.087 76	65.4804	5.612	0.3118
63.1282	0.1013	64.4872	0.087 60	66.2368	5.585	0.4155

[a] Thermal diffusivity values were adjusted by factors k_f.

Table 9. Experimental Data for 3,3-Dimethylpentane: Means of the A and C Results[a]

ϑ_0/°C	p_0/MPa	ϑ_λ/°C	λ/W·m^{-1}·K^{-1}	ϑ_κ/°C	$\kappa/10^{-8}$ m^2·s^{-1}	$(Q_0/4\pi\lambda)$/K
22.3858	0.1013	22.8817	0.100 59	23.5378	6.6576	0.1547
22.3851	0.1013	23.2356	0.100 36	24.3667	6.6828	0.2605
22.3863	0.1013	23.4837	0.100 20	24.9316	6.5949	0.3476
22.3857	0.1013	22.8629	0.100 49	23.4884	6.5918	0.1532
−17.5320	0.1013	−17.0358	0.111 58	−16.3269	7.8020	0.1311
−17.5307	0.1013	−16.7051	0.111 34	−15.5311	7.7558	0.2202
−17.5276	0.1013	−16.4399	0.111 16	−14.8996	7.7061	0.2935
2.5167	0.1013	3.0217	0.105 99	3.7179	7.2520	0.1424
2.5148	0.1013	3.3485	0.105 82	4.4921	7.1986	0.2385
2.5153	0.1013	3.6280	0.105 70	5.1529	7.1766	0.3197
42.7169	0.1013	43.2302	0.095 28	43.8969	6.2160	0.1683
42.7176	0.1013	43.5216	0.094 99	44.5530	6.0854	0.2802
42.7179	0.1013	43.7829	0.094 81	45.1476	6.0522	0.3754
60.1162	0.1013	60.6032	0.090 74	61.2186	5.7427	0.1785
60.1170	0.1013	60.9517	0.090 63	62.0076	5.7585	0.3015
60.1163	0.1013	61.2220	0.090 47	62.6206	5.7418	0.4008

[a] Thermal diffusivity values were adjusted by factors k_f.

Table 10. Experimental Data for 2,4-Dimethylpentane: Means of the B and D Results[a]

ϑ_0/°C	p_0/MPa	ϑ_λ/°C	λ/W·m^{-1}·K^{-1}	ϑ_κ/°C	$\kappa/10^{-8}$ m^2·s^{-1}	$(Q_0/4\pi\lambda)$/K
22.3862	0.1013	23.0408	0.102 47	24.0260	6.904	0.1494
22.3859	0.1013	23.4761	0.102 19	25.1022	6.835	0.2523
22.3866	0.1013	23.8172	0.102 00	25.9324	6.772	0.3358
−17.1549	0.1013	−16.5554	0.113 82	−15.5903	7.905	0.1269
−17.1540	0.1013	−16.1610	0.113 49	−14.5729	7.839	0.2123
−17.1528	0.1013	−15.8481	0.113 33	−13.7838	7.760	0.2832
2.5146	0.1013	3.1491	0.108 16	4.1402	7.417	0.1387
2.5141	0.1013	3.5435	0.107 87	5.1166	7.289	0.2319
2.5153	0.1013	3.8934	0.107 66	6.0107	7.283	0.3089
42.7174	0.1013	43.4023	0.096 92	44.3979	6.428	0.1628
42.7194	0.1013	43.8624	0.096 68	45.5190	6.394	0.2732
42.7162	0.1013	44.2225	0.096 45	46.3816	6.321	0.3667
60.1160	0.1013	60.8112	0.092 40	61.7835	5.993	0.1747
60.1162	0.1013	61.2800	0.092 13	62.9067	5.979	0.2919
60.1158	0.1013	61.6634	0.091 97	63.8220	5.955	0.3899

[a] Thermal diffusivity values were adjusted by factors k_f.

The heat energy may be transported by phonon mechanisms in electrically nonconductive liquids. Then the thermal conductivity λ and thermal diffusivity κ are obtained from the kinetic theory of gas as follows:

$$\lambda = (1/3)c_p\rho\tilde{u}\tilde{l} \tag{11a}$$

$$\kappa = \lambda/c_p\rho = (1/3)\tilde{u}\tilde{l} \tag{11b}$$

where $\tilde{u}$ is the propagation (mean) velocity of the phonon and $\tilde{l}$ is the mean free path of the phonon. Figure 9 shows the values of thermal conductivity, thermal diffusivity, and volumic heat capacity at 298.15 K against the velocity of sound from the literature,[14−18] taken as the phonon velocity for heat transfer, although the velocity of sound depends on the frequency when measured. For the normal alkanes, thermal conductivity and thermal diffusivity form a line similar to the case of Figure 6 (also Figure 7), and the volumic heat capacities of all alkanes are clearly in a straight line. The apparent mean free path $\tilde{l}$ is calculated using eq 11b (Figure 10), which may indicate a spatial roughness factor disturbing the heat transfer.

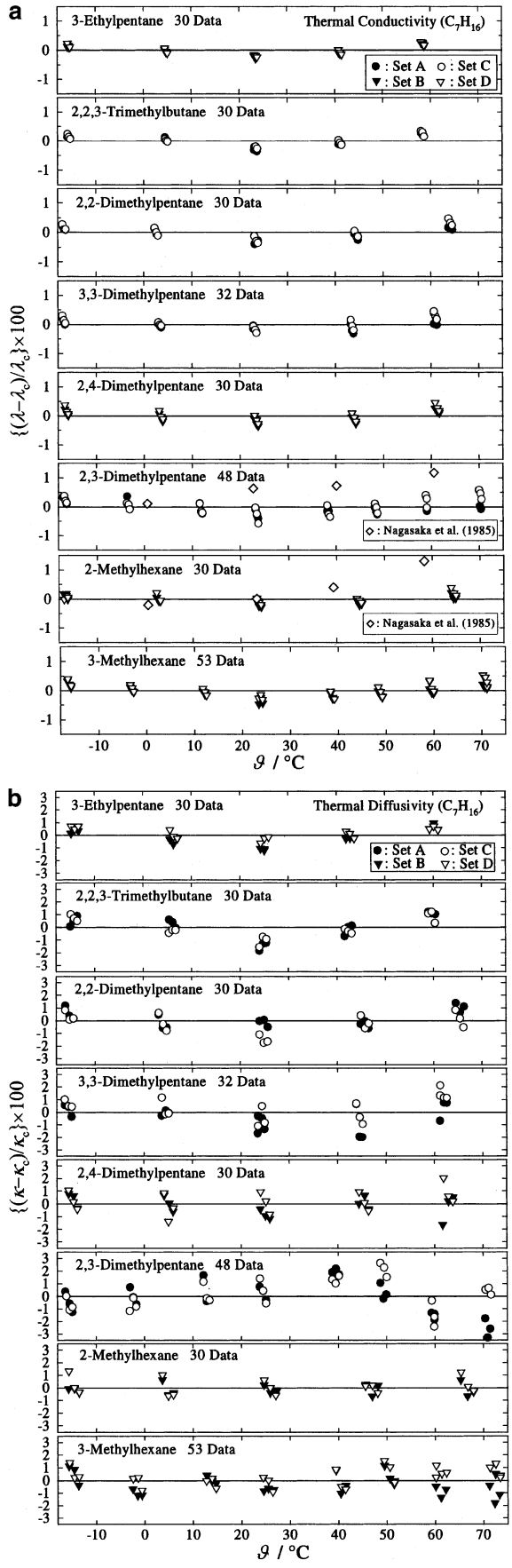

Figure 4. Deviations of measured values from the formulas (eqs 8 and 9 with coefficients listed in Table 2) respectively fitted for eight isomers of C_7H_{16} together with literature values:[8] (a) thermal conductivity; (b) thermal diffusivity. Values were adjusted by factors k_f.

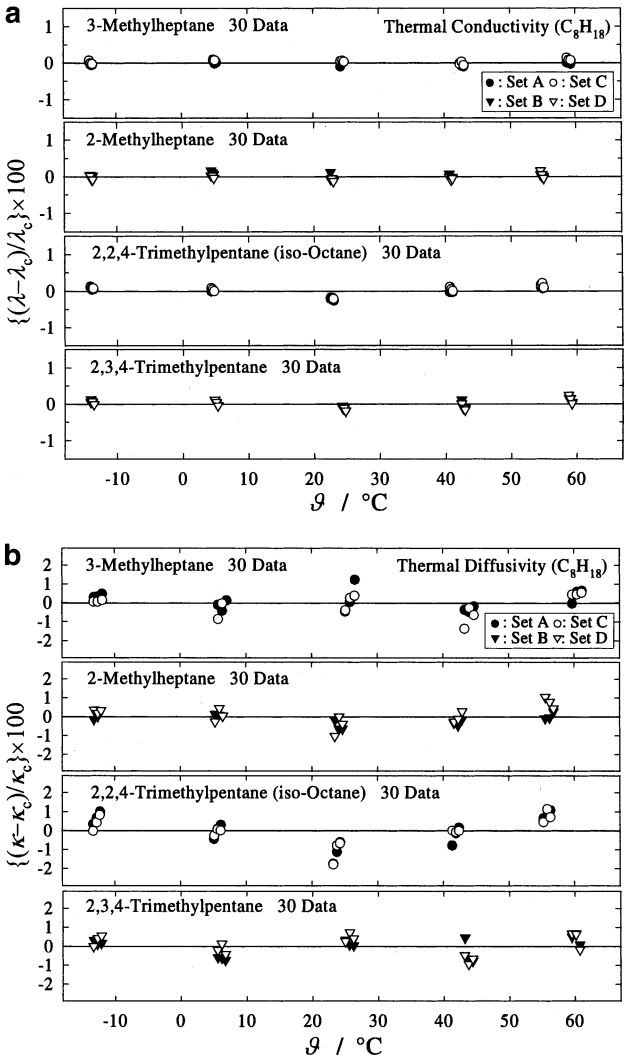

Figure 5. Deviations of measured values from the formulas (eqs 8 and 9 with coefficients listed in Table 2) respectively fitted for four isomers of C_8H_{18}: (a) thermal conductivity; (b) thermal diffusivity. Values were adjusted by factors k_f.

Evaluations of Uncertainty. The evaluation of the uncertainty components in the measurement is made using the simplified working formula

$$\Delta T = (Q_0/4\pi\lambda)\ln(t/\mathrm{s}) + (Q_0/4\pi\lambda)\ln(4\kappa\mathrm{s}/a^2\mathrm{C}) \quad (12)$$

The uncertainty in the thermal conductivity can be evaluated as[1,3]

$$\frac{\delta\lambda}{\lambda} = \frac{\delta Q_0}{Q_0} + \frac{\delta(\mathrm{d}R_W/\mathrm{d}T)}{\mathrm{d}R_W/\mathrm{d}T} + \frac{\delta(\Delta T_f - \Delta T_i)}{\Delta T_f - \Delta T_i} + \frac{\delta\tau(t_f - t_i)}{t_f t_i \ln(t_f/t_i)} + \left(\frac{\delta\lambda}{\lambda}\right)_{\text{sample}} + \left(\frac{\delta\lambda}{\lambda}\right)_{\text{pressure}} + \left(\frac{\delta\lambda}{\lambda}\right)_{\text{others}} \quad (13)$$

where $\delta(*)$ is the uncertainty of the terms (*), R_W is the resistance of the hot-wire sensor, and $\delta\tau$ is the ambiguity of the time lag of both trigger signals to the bridge and the digital voltmeter. The magnitude of the respective components, contributing as a random or systematic part, is the same as that in the previous study.[2,3] The first component is 0.17%, in terms of the standard uncertainty (as a random part; type A), the second is ≈0.05% (as a systematic part; type A), the third is ≈0.05% (as a random

Table 11. Experimental Data for 2,3-Dimethylpentane: Means of the A and C Results[a]

ϑ_0/°C	p_0/MPa	ϑ_λ/°C	λ/W·m^{-1}·K^{-1}	ϑ_κ/°C	$\kappa/10^{-8}$ m^2·s^{-1}	$(Q_0/4\pi\lambda)$/K
22.7267	0.1013	23.2051	0.106 31	23.8479	7.164	0.1479
22.7276	0.1013	23.4974	0.106 02	24.5278	7.101	0.2422
22.7270	0.1013	23.7568	0.105 71	25.1281	7.023	0.3321
−4.0236	0.1013	−3.5831	0.114 00	−2.9733	7.799	0.1288
−4.0212	0.1013	−3.2779	0.113 70	−2.2486	7.789	0.2165
−4.0203	0.1013	−3.0310	0.113 48	−1.6675	7.724	0.2933
−17.2945	0.1013	−16.8478	0.117 76	−16.2159	8.193	0.1242
−17.1683	0.1013	−16.4539	0.117 48	−15.4524	8.088	0.2041
−17.1662	0.1013	−16.2026	0.117 31	−14.8542	8.053	0.2773
11.1228	0.1013	11.5902	0.109 69	12.2320	7.508	0.1373
11.1235	0.1013	11.8738	0.109 31	12.8896	7.366	0.2307
11.1236	0.1013	12.1233	0.109 18	13.4763	7.347	0.3083
37.7186	0.1013	38.1919	0.102 22	38.8202	6.789	0.1532
37.7191	0.1013	38.5079	0.101 98	39.5488	6.768	0.2569
37.7194	0.1013	38.7805	0.101 76	40.1802	6.755	0.3454
47.6750	0.1013	48.1463	0.099 59	48.7598	6.529	0.1605
47.6744	0.1013	48.4402	0.099 37	49.4344	6.459	0.2683
47.6743	0.1013	48.6979	0.099 16	50.0252	6.430	0.3613
58.3949	0.1013	58.8098	0.097 00	59.3493	6.072	0.1657
58.3955	0.1013	59.0602	0.096 62	59.9138	6.001	0.2774
58.3954	0.1013	59.0591	0.096 51	59.9103	5.991	0.2780
69.5654	0.1013	69.9688	0.094 11	70.4933	5.784	0.1749
69.5649	0.1013	70.2099	0.093 73	71.0459	5.723	0.2905
69.5650	0.1013	70.4429	0.093 53	71.5777	5.719	0.3926

[a] Thermal diffusivity values were adjusted by factors k_f.

Table 12. Experimental Data for 2-Methylhexane: Means of the B and D Results[a]

ϑ_0/°C	p_0/MPa	ϑ_λ/°C	λ/W·m^{-1}·K^{-1}	ϑ_κ/°C	$\kappa/10^{-8}$ m^2·s^{-1}	$(Q_0/4\pi\lambda)$/K
22.5622	0.1013	23.3141	0.110 95	24.6492	7.500	0.1401
22.5633	0.1013	23.7843	0.110 65	25.9255	7.425	0.2303
22.5632	0.1013	24.2483	0.110 46	27.1878	7.381	0.3196
−17.5644	0.1013	−16.9070	0.122 68	−15.6874	8.412	0.1182
−17.5644	0.1013	−16.4840	0.122 64	−14.5037	8.332	0.1966
−17.5639	0.1013	−16.1294	0.122 39	−13.5132	8.283	0.2624
1.7081	0.1013	2.4066	0.117 17	3.6793	7.998	0.1273
1.7083	0.1013	2.8577	0.116 82	4.9087	7.858	0.2140
1.7081	0.1013	3.2399	0.116 70	5.9736	7.845	0.2853
43.4595	0.1013	44.2543	0.104 93	45.6212	7.017	0.1521
43.4601	0.1013	44.7725	0.104 65	47.0103	6.957	0.2534
43.4598	0.1013	45.2045	0.104 52	48.1762	6.939	0.3374
63.1288	0.1013	63.9518	0.099 56	65.3384	6.628	0.1601
63.1285	0.1013	64.4992	0.099 20	66.7642	6.516	0.2721
63.1288	0.1013	64.9582	0.099 05	67.9716	6.491	0.3644

[a] Thermal diffusivity values were adjusted by factors k_f.

part; type A), and the fourth is negligible. The fifth (the sample material) is rather difficult to estimate, because of the lack of exact information about purity. However, most of the impurities are thought to be isomers that are difficult to separate from the sample material, owing to their boiling temperatures approaching each other. The thermal properties of such isomers are naturally close to those of the sample, and their purities are expected to be less than 2% (although a few substances such as 3-ethylpentane and 3-methylheptane contain certainly extra impurity [this means other isomers]). The dissolved content of water is expected to be adequately small to the limit of not affecting more than the uncertainty of measurement, owing to the alkane's hydrophobic peculiarity. The effect of dissolved air on thermal properties has not been precisely known, but it may not be due to molar fraction but partial molar density. The molar concentration (partial molar density) of air is estimated to be roughly (5 to 15) $\times$ 10^{-6} mol/m^3 [molar fraction, (15 to 20) $\times$ 10^{-4}] in saturation when the partial pressure is 101.3 kPa.[7] This value is about one digit larger than that of water. It might not be appropriate to refer to the effect of air dissolved in water, but the air solution (whose concentration is 0.746 $\times$ 10^{-6} mol/m^3 in saturation [molar fraction, 0.134 $\times$ 10^{-4}]) makes the density (as one of the thermophysical properties) smaller by 2.9 parts per million at 25 °C.[20] Judging from this result, the dissolved air may not have a remarkable effect on thermal properties larger than 0.01%. Therefore, this term is assumed to be ≈0.10%, excluding substances such as 3-ethylpentane and 3-methylheptane (as a random part; type B). The sixth term (the variation of pressure) is neglected because the inside communicates with the outside (atmosphere) via a capillary before starting a measurement and then the pressure dependence $(1/\lambda)(\partial\lambda/\partial p)_T$ is small [(≈3 to 5) $\times$ 10^{-3}]/MPa. At last, the other components, including the potential lead, the sampling time-step distribution, and so forth, have an effect of ≈0.04% (a random part; mixed types A and B). Overall, the combined standard uncertainty is about 0.24%, evaluated as the root sum square of the various components (excluding 3-ethylpentane and 3-methylheptane, and their uncertainty may be estimated as about 0.34%).

For measurement of the thermal diffusivity, the original uncertainty $(2\delta a/a)$ is replaced by the term $(\delta\kappa/\kappa)_{cal} = (\delta k_f/$

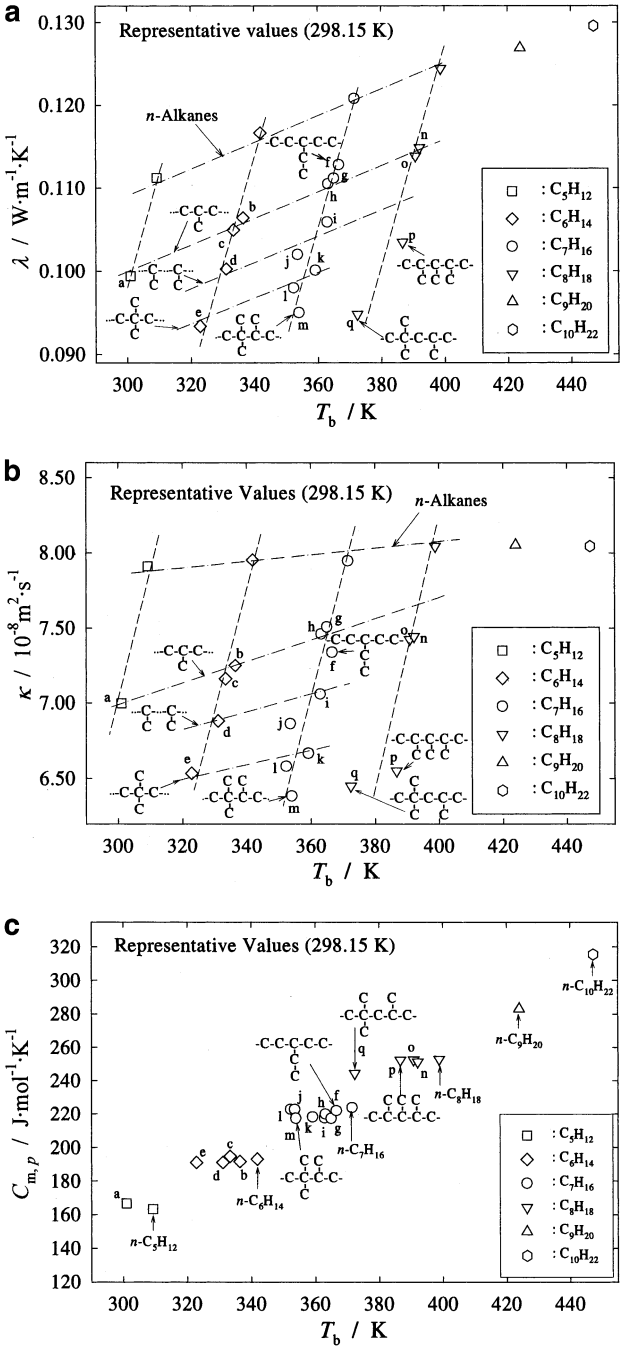

Figure 6. Values calculated at 298.15 K versus the boiling point[9] together with those of *n*-alkanes and isopentane.[3] Materials and symbols are designated as follows: C_5H_{12} (a, isopentane); C_6H_{14} (b, 3-methylpentane; c, 2-methylpentane; d, 2,3-dimethylbutane; e, 2,2-dimethylbutane); C_7H_{16} (f, 3-ethylpentane; g, 3-methylhexane; h, 2-methylhexane; i, 2,3-dimethylpentane; j, 2,4-dimethylpentane; k, 3,3-dimethylpentane; l, 2,2-dimethylpentane; m, 2,2,3-trimethylbutane); C_8H_{18} (n, 3-methylheptane; o, 2-methylheptane; p, 2,3,4-trimethylpentane; q, 2,2,4-trimethylpentane [isooctane]). (a) Thermal conductivity; (b) thermal diffusivity. Values were adjusted by factors k_f. (c) Molar heat capacity.

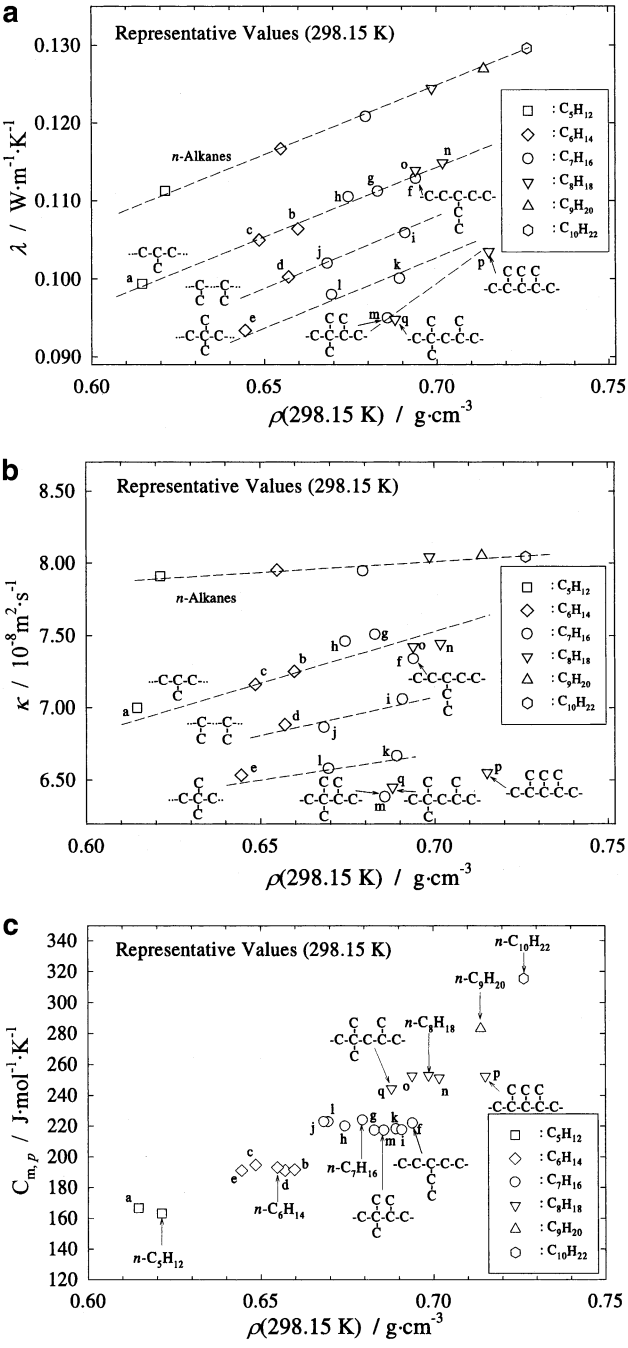

Figure 7. Values calculated at 298.15 K versus the density[9] together with those of *n*-alkanes and isopentane.[3] Materials and symbols are designated as follows: C_5H_{12} (a, isopentane); C_6H_{14} (b, 3-methylpentane; c, 2-methylpentane; d, 2,3-dimethylbutane; e, 2,2-dimethylbutane); C_7H_{16} (f, 3-ethylpentane; g, 3-methylhexane; h, 2-methylhexane; i, 2,3-dimethylpentane; j, 2,4-dimethylpentane; k, 3,3-dimethylpentane; l, 2,2-dimethylpentane; m, 2,2,3-trimethylbutane); C_8H_{18} (n, 3-methylheptane; o, 2-methylheptane; p, 2,3,4-trimethylpentane; q, 2,2,4-trimethylpentane [isooctane]). (a) Thermal conductivity; (b) thermal diffusivity. Values were adjusted by factors k_f. (c) Molar heat capacity.

k_f), since substantial correction of the diameters of the wire have been made for respective configurations, and the uncertainty is evaluated as follows:[1,3]

$$\delta\kappa/\kappa = (\delta\kappa/\kappa)_{cal} + \delta(\Delta T)_0/(Q_0/4\pi\lambda) + (\delta\lambda/\lambda)^* \ln(4\kappa s/a^2 C) + (\delta\kappa/\kappa)_{material} \quad (14)$$

In this formula, the first term cannot be evaluated precisely but can tentatively be said to be 0.3% (a systematic part; type B), and the second term [$\delta(\Delta T)_0$, the initially remaining deflection in terms of temperature, originating from an inadequate balance in the bridge at temperature T_0] is about 0.5% (a random part; type B). According to the third term, subcomponents $\delta Q_0/Q_0$ and $(\delta\lambda/\lambda)_{material}$ in eq 14 do not practically affect $\delta\kappa/\kappa$, and therefore, $(\delta\lambda/\lambda)^*$ is 0.084%.

Table 13. Experimental Data for 3-Methylhexane: Means of the B and D Results[a]

ϑ_0/°C	p_0/MPa	ϑ_λ/°C	λ/W·m^{-1}·K^{-1}	ϑ_κ/°C	$\kappa/10^{-8}$ m^2·s^{-1}	$(Q_0/4\pi\lambda)$/K
22.7276	0.1013	23.3993	0.111 26	24.4715	7.499	0.1425
22.7268	0.1013	23.7969	0.111 33	25.4983	7.472	0.2284
22.7273	0.1013	24.1998	0.111 02	26.5236	7.410	0.3175
−4.0243	0.1013	−3.4299	0.119 56	−2.4490	8.144	0.1222
−4.0225	0.1013	−3.0388	0.119 32	−1.4216	8.102	0.2033
−4.0211	0.1013	−2.7107	0.119 11	−0.5714	8.041	0.2734
−17.1118	0.1013	−16.5373	0.123 58	−15.5587	8.588	0.1139
−17.1084	0.1013	−16.1483	0.123 28	−14.5219	8.502	0.1922
−17.0597	0.1013	−15.7710	0.123 08	−13.6068	8.429	0.2608
11.1232	0.1013	11.7494	0.115 05	12.7690	7.815	0.1302
11.1231	0.1013	12.1655	0.114 79	13.8583	7.780	0.2176
11.1241	0.1013	12.5066	0.114 61	14.7352	7.722	0.2914
37.7205	0.1013	38.3911	0.107 30	39.4499	7.220	0.1435
37.7223	0.1013	38.8195	0.106 96	40.5142	7.081	0.2418
37.7200	0.1013	39.1854	0.106 82	41.4515	7.074	0.3226
47.6744	0.1013	48.3733	0.104 55	49.4652	7.015	0.151
47.6744	0.1013	48.8252	0.104 25	50.6030	6.936	0.2524
47.6744	0.1013	49.1947	0.104 04	51.5137	6.856	0.3394
47.6742	0.1013	49.1920	0.104 00	51.5149	6.869	0.3373
58.3941	0.1013	59.0924	0.101 65	60.1480	6.685	0.1571
58.3943	0.1013	59.5411	0.101 28	61.2554	6.611	0.2621
58.3935	0.1013	59.9363	0.101 11	62.2485	6.611	0.3513
69.5653	0.1013	70.2698	0.098 57	71.3069	6.417	0.1631
69.5654	0.1013	70.7375	0.098 31	72.4600	6.370	0.2731
69.5664	0.1013	71.1503	0.098 07	73.4673	6.369	0.3691
69.5660	0.1013	71.1285	0.098 13	73.4053	6.318	0.3687

[a] Thermal diffusivity values were adjusted by factors k_f.

Table 14. Experimental Data for 3-Ethylpentane: Means of the B and D Results[a]

ϑ_0/°C	p_0/MPa	ϑ_λ/°C	λ/W·m^{-1}·K^{-1}	ϑ_κ/°C	$\kappa/10^{-8}$ m^2·s^{-1}	$(Q_0/4\pi\lambda)$/K
22.4987	0.1013	23.1809	0.113 172	24.3329	7.290	0.1340
22.4988	0.1013	23.4708	0.113 031	25.1130	7.281	0.1909
22.4989	0.1013	23.6291	0.112 959	25.5414	7.279	0.2216
−16.4808	0.1013	−15.8748	0.125 323	−14.7867	8.276	0.1126
−16.4770	0.1013	−15.6060	0.125 173	−14.0413	8.264	0.1619
−16.4714	0.1013	−15.3237	0.125 066	−13.2636	8.249	0.2135
3.8251	0.1013	4.4723	0.119 049	5.6029	7.781	0.1232
3.8245	0.1013	4.7429	0.118 844	6.3362	7.729	0.1762
3.8260	0.1013	5.0399	0.118 72	7.1473	7.721	0.2328
40.0826	0.1013	40.8064	0.108 059	42.0119	6.952	0.1436
40.0824	0.1013	41.1189	0.107 891	42.8407	6.928	0.2062
40.0828	0.1013	41.4325	0.107 752	43.6652	6.896	0.2699
57.3182	0.1013	58.0712	0.103 186	59.2978	6.591	0.1523
57.3208	0.1013	58.4103	0.103 057	60.1898	6.594	0.2197
57.3208	0.1013	58.7419	0.102 874	61.0460	6.548	0.2889

[a] Thermal diffusivity values were adjusted by factors k_f.

Table 15. Experimental Data for 2,2,4-Trimethylpentane: Means of the A and C Results[a]

ϑ_0/°C	p_0/MPa	ϑ_λ/°C	λ/W·m^{-1}·K^{-1}	ϑ_κ/°C	$\kappa/10^{-8}$ m^2·s^{-1}	$(Q_0/4\pi\lambda)$/K
21.9767	0.1013	22.5161	0.095 16	23.2561	6.373	0.1439
21.9773	0.1013	22.7478	0.095 09	23.8136	6.414	0.2020
21.9766	0.1013	22.9514	0.095 02	24.3039	6.423	0.2542
−14.5704	0.1013	−14.0431	0.104 17	−13.2621	7.300	0.1252
−14.5701	0.1013	−13.8262	0.104 06	−12.7194	7.317	0.1753
−14.5698	0.1013	−13.6313	0.104 01	−12.2294	7.332	0.2200
3.8263	0.1013	4.3660	0.099 71	5.1386	6.860	0.1343
3.8259	0.1013	4.5911	0.099 66	5.6916	6.878	0.1890
3.8258	0.1013	4.7835	0.099 58	6.1617	6.873	0.2364
40.0620	0.1013	40.6351	0.091 08	41.4082	6.066	0.1560
40.0631	0.1013	40.8656	0.091 00	41.9506	6.071	0.2175
40.0626	0.1013	41.0659	0.090 93	42.4238	6.072	0.2713
53.9533	0.1013	54.5416	0.087 86	55.3229	5.818	0.1635
53.9524	0.1013	54.7813	0.087 80	55.8854	5.827	0.2290
53.9518	0.1013	54.9884	0.087 71	56.3677	5.814	0.2872

[a] Thermal diffusivity values were adjusted by factors k_f.

This term is estimated to be 0.67% [$\ln(4\kappa s/a^2C) \approx 8$] (a random part; type A). The last term $(\delta\kappa/\kappa)_{material}$ is actually the same as $(\delta\lambda/\lambda)_{material}$ and is 0.10% (a random part; type B). Finally, the overall uncertainty is estimated to be 0.90%, computed as the root sum square of the subcomponents (including 3-ethylpentane and 3-ethylheptane).

Table 16. Experimental Data for 2,3,4-Trimethylpentane: Means of the B and D Results[a]

ϑ_0/°C	p_0/MPa	ϑ_λ/°C	λ/W·m^{-1}·K^{-1}	ϑ_κ/°C	$\kappa/10^{-8}$ m^2·s^{-1}	$(Q_0/4\pi\lambda)$/K
23.5972	0.1013	24.1810	0.103 59	25.0122	6.569	0.1456
23.5959	0.1013	24.4350	0.103 48	25.6306	6.564	0.2091
23.5971	0.1013	24.6939	0.103 34	26.2530	6.540	0.2746
−14.6291	0.1013	−14.0874	0.112 69	−13.2757	7.320	0.1266
−14.6290	0.1013	−13.8582	0.112 61	−12.7021	7.316	0.1800
−14.6281	0.1013	−13.6144	0.112 48	−12.0920	7.311	0.2363
4.2485	0.1013	4.7980	0.108 31	5.5945	6.907	0.1344
4.2490	0.1013	5.0448	0.108 17	6.2006	6.905	0.1941
4.2492	0.1013	5.2855	0.108 03	6.7847	6.871	0.2547
41.7803	0.1013	42.3758	0.099 48	43.1965	6.189	0.1562
41.7805	0.1013	42.6156	0.099 26	43.7556	6.123	0.2233
41.7805	0.1013	42.8839	0.099 16	44.3921	6.121	0.2945
58.1083	0.1013	58.7169	0.095 80	59.5383	5.900	0.1645
58.1078	0.1013	58.9840	0.095 68	60.1665	5.892	0.2369
58.1071	0.1013	59.2429	0.095 51	60.7645	5.839	0.3124

[a] Thermal diffusivity values were adjusted by factors k_f.

Table 17. Experimental Data for 2-Methylheptane: Means of the B and D Results[a]

ϑ_0/°C	p_0/MPa	ϑ_λ/°C	λ/W·m^{-1}·K^{-1}	ϑ_κ/°C	$\kappa/10^{-8}$ m^2·s^{-1}	$(Q_0/4\pi\lambda)$/K
21.9766	0.1013	22.5669	0.114 55	23.5381	7.409	0.1200
21.9758	0.1013	22.7980	0.114 41	24.1557	7.418	0.1665
21.9757	0.1013	23.0069	0.114 28	24.7043	7.392	0.2096
−14.5696	0.1013	−14.0340	0.124 38	−13.1054	8.228	0.1035
−14.5700	0.1013	−13.8215	0.124 24	−12.5234	8.216	0.1447
−14.5698	0.1013	−13.6429	0.124 20	−12.0316	8.224	0.1788
3.8265	0.1013	4.3843	0.119 52	5.3287	7.830	0.1103
3.8268	0.1013	4.6167	0.119 43	5.9595	7.842	0.1555
3.8274	0.1013	4.8132	0.119 30	6.4832	7.814	0.1948
40.0644	0.1013	40.6830	0.109 70	41.6810	7.054	0.1280
40.0638	0.1013	40.9232	0.109 55	42.3099	7.042	0.1778
40.0639	0.1013	41.1482	0.109 51	42.9034	7.055	0.2235
53.9516	0.1013	54.5945	0.106 05	55.6221	6.816	0.1338
53.9512	0.1013	54.8531	0.105 90	56.2915	6.795	0.1883
53.9509	0.1013	55.0758	0.105 79	56.8678	6.781	0.2352

[a] Thermal diffusivity values were adjusted by factors k_f.

Table 18. Experimental Data for 3-Methylheptane: Means of the A and C Results[a]

ϑ_0/°C	p_0/MPa	ϑ_λ/°C	λ/W·m^{-1}·K^{-1}	ϑ_κ/°C	$\kappa/10^{-8}$ m^2·s^{-1}	$(Q_0/4\pi\lambda)$/K
23.5994	0.1013	24.2115	0.115 05	25.1689	7.409	0.1332
23.5942	0.1013	24.4767	0.115 04	25.8653	7.436	0.1905
23.5983	0.1013	24.7636	0.114 97	26.6105	7.468	0.2493
−14.6295	0.1013	−14.0672	0.125 47	−13.1360	8.290	0.1151
−14.6293	0.1013	−13.8285	0.125 31	−12.5021	8.276	0.1640
−14.6286	0.1013	−13.5746	0.125 22	−11.8273	8.271	0.2157
4.2507	0.1013	4.8449	0.120 40	5.7970	7.825	0.1261
4.2497	0.1013	5.0833	0.120 28	6.4231	7.831	0.1763
4.2502	0.1013	5.2186	0.120 25	6.7800	7.844	0.2040
41.7803	0.1013	42.4106	0.110 15	43.3656	6.982	0.1422
41.7802	0.1013	42.6892	0.110 07	44.0732	7.002	0.2037
41.7806	0.1013	42.9703	0.109 93	44.7791	6.984	0.2672
58.1092	0.1013	58.7769	0.105 84	59.7762	6.700	0.1521
58.1085	0.1013	59.0605	0.105 74	60.4891	6.705	0.2161
58.1080	0.1013	59.3582	0.105 63	61.2330	6.694	0.2841

[a] Thermal diffusivity values were adjusted by factors k_f.

Discussion and Conclusions

The original data on the thermal conductivity and thermal diffusivity for the 16 isomers of the alkane C_nH_{2n+2} ($n = 6$ to 8) are reported. The various (volumic, $c_p\rho$; specific, c_p; and molar, $C_{m,p}$) heat capacities were derived at the nominal temperature 298.15 K from the ratio of the thermal conductivity to the thermal diffusivity λ/κ, the density ρ, and the molar mass M.[9] The derived c_p (or $C_{m,p}$) seems consistent with values from the literature[7,9] within about 1%. The thermal properties were graphically illustrated with the boiling point T_b and the density ρ, and some clear relevancies were found between transport properties (λ and κ) and T_b or ρ, and also molecular configuration. Further, when understanding the heat conduction mechanism, we had better recognize that the primary properties are the thermal diffusivity κ and volumic heat capacity $c_p\rho$, and the thermal conductivity λ is the secondary one derived from the value $\kappa c_p\rho$.

In conclusion, empirical equations for the thermal conductivity and thermal diffusivity of liquid alkane are reported, with an uncertainty of 0.5% for the thermal conductivity and 1.8% for the thermal diffusivity and the heat capacity (respectively, with a level $k_p = 2$, $p = 95\%$), although that of thermal conductivity may be inferior for a few substances (such as 3-ethylpentane and 3-methylheptane) containing comparatively larger impurities (i.e.

Table 19. Comparison of the Present Data at 298.15 K and 101.325 kPa with the Reference Data of the Molar Heat Capacity and the Velocity of Sound (u/m·s^{-1})

material	M / g·mol^{-1}	ϑ_b / °C	λ / W·m^{-1}·K^{-1}	κ / 10^{-8} m^2·s^{-1}	$c_p\rho$ / MJ·m^{-3}·K^{-1}	c_p / kJ·kg^{-1}·K^{-1}	$C_{m,p}$ / J·mol^{-1}·K^{-1}	ρ / kg·m^{-3}	$(d\lambda/dT)/\lambda$ / 10^{-3} K^{-1}	$(d\kappa/dT)/\kappa$ / 10^{-3} K^{-1}	$C_{m,p}$(ref) / J·mol^{-1}·K^{-1}	u(ref) / m·s^{-1}
isopentane[3]	72.151[a]	27.844[a]	0.099 37	6.998	1.420	2.310	166.7	614.62[a]	−3.50	−3.94	164.90[b]	991.0[c]
n-pentane[3]	72.151[a]	36.065[a]	0.111 25	7.910	1.407	2.264	163.4	621.30[a]	−3.40	−3.29	171.50[b]	1010.6[c]
2,2-dimethylbutane	86.178[a]	49.741[a]	0.093 36	6.534	1.429	2.217	191.1	644.46[a]	−3.11	−3.73	188.70[a]	1006.5[d]
2,3-dimethylbutane	86.178[a]	57.988[a]	0.100 26	6.882	1.457	2.218	191.2	657.02[a]	−2.92	−3.34	188.70[a]	1046.6[d,e]
2-methylpentane	86.178[a]	60.271[a]	0.104 97	7.160	1.466	2.261	194.8	648.52[a]	−2.96	−3.50	193.91[a]	1041.4[d,e]
3-methylpentane	86.178[a]	63.282[a]	0.106 40	7.249	1.468	2.225	191.7	659.76[a]	−2.92	−3.43	190.67[a]	1071.4[d,e]
n-hexane[3]	86.178[a]	68.740[a]	0.116 68	7.952	1.467	2.241	193.1	654.84[a]	−2.87	−2.87	195.48[a]	1076.9[c,e]
2,2,3-trimethylbutane	100.206[a]	80.856[a]	0.094 96	6.385	1.487	2.170	217.4	685.64[a]	−2.57	−3.36	213.60[a]	1080.0[c]
2,2-dimethylpentane	100.206[a]	79.168[a]	0.097 96	6.580	1.489	2.224	222.8	669.48[a]	−2.71	−3.73	221.20[a]	1065.0[f]
3,3-dimethylpentane	100.206[a]	86.037[a]	0.100 08	6.667	1.501	2.178	218.3	689.16[a]	−2.67	−3.90	214.77[a]	1115.0[f]
2,4-dimethylpentane	100.206[a]	80.472[a]	0.101 99	6.863	1.486	2.224	222.9	668.23[a]	−2.71	−3.49	224.30[a]	1068.0[f]
2,3-dimethylpentane	100.206[a]	89.757[a]	0.105 90	7.058	1.500	2.172	217.6	690.81[a]	−2.59	−3.85	218.28[a]	1133.0[f]
2-methylhexane	100.206[a]	90.027[a]	0.110 50	7.460	1.481	2.197	220.1	674.34[a]	−2.61	−2.97	222.94[a]	1098.8[c]
3-methylhexane	100.206[a]	91.848[a]	0.111 21	7.508	1.481	2.169	217.4	682.88[a]	−2.58	−3.20		1147.7[c]
3-ethylpentane	100.206[a]	93.475[a]	0.112 84	7.337	1.538	2.216	222.1	693.92[a]	−2.66	−3.09	219.60[a]	1149.9[c]
n-heptane[3]	100.206[a]	98.403[a]	0.120 69	7.920	1.524	2.243	224.7*	679.46[a]	−2.64	−2.90	224.74[b]	1129.8[e]
2,2,4-trimethylpentane	114.233[a]	99.236[a]	0.094 77	6.450	1.469	2.136	244.0	687.84[a]	−2.51	−3.40	239.00[a]	1081.9[g]
2,3,4-trimethylpentane	114.233[a]	113.472[a]	0.103 47	6.550	1.580	2.209	252.4	715.09[a]	−2.25	−3.02	248.60[a]	
2-methylheptane	114.233[a]	117.654[a]	0.113 88	7.424	1.534	2.211	252.5	693.87[a]	−2.35	−2.81	251.99[a]	
3-methylheptane	114.233[a]	118.970[a]	0.114 88	7.444	1.543	2.199	251.2	701.73[a]	−2.35	−2.93	250.20[a]	
n-octane[3]	114.233[a]	125.670[a]	0.124 40	8.044	1.547	2.214	252.9	698.62[a]	−2.36	−2.38	254.15[a]	1172.2[e]
n-nonane[3]	128.260[a]	150.798[a]	0.126 91	8.053	1.576	2.208	283.2	713.75[a]	−2.15	−2.18	284.45[a]	1206.4[e]
n-decane[3]	142.287[a]	174.123[a]	0.129 57	8.044	1.611	2.218	315.5	726.35[a]	−1.98	−1.80	314.54[a]	1234.5[e]
toluene[3]	92.142[a]	110.630[a]	0.130 51	9.060	1.441	1.671	154.0	862.2[a]	−2.18	−2.26	157.29[a]	1304.7[e]

* Referenced value for calibration. [a] Referred from *TRC Table*.[9] [b] Referred to Kagaku Binran.[7] [c] Referred from Landolt−Börnstein table.[14] [d] Referred from Tamura et al.[17] [e] Tardajos et al.[15] [f] Referred from Awwad et al.[16] [g] Referred from Nath.[18,19]

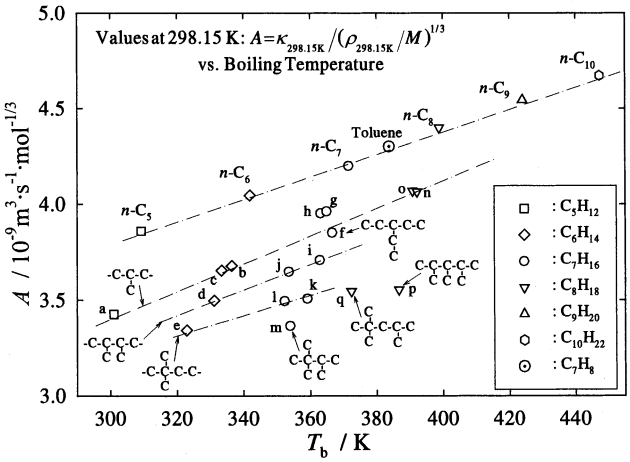

Figure 8. Values $A = \kappa/(\rho/M)^{1/3}$ calculated at 298.15 K versus the boiling point T_b, together with those of *n*-alkanes, isopentane, and toluene.[3] Materials and symbols are designated as follows: C_5H_{12} (a, isopentane); C_6H_{14} (b, 3-methylpentane; c, 2-methylpentane; d, 2,3-dimethylbutane; e, 2,2-dimethylbutane); C_7H_{16} (f, 3-ethylpentane; g, 3-methylhexane; h, 2-methylhexane; i, 2,3-dimethylpentane; j, 2,4-dimethylpentane; k, 3,3-dimethylpentane; l, 2,2-dimethylpentane; m, 2,2,3-trimethylbutane); C_8H_{18} (n, 3-methylheptane; o, 2-methylheptane; p, 2,3,4-trimethylpentane; q, 2,2,4-trimethylpentane [isooctane]). Thermal diffusivity κ was adjusted by factors k_f.

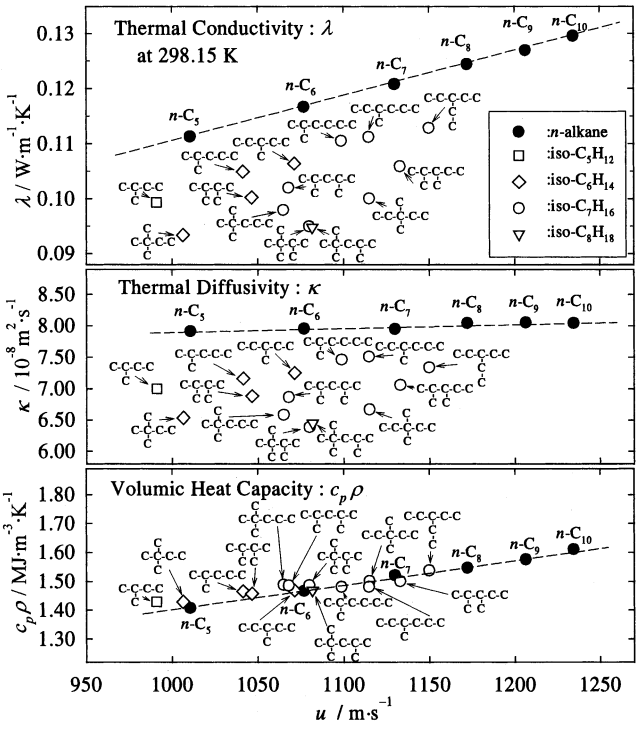

Figure 9. Thermal conductivity, thermal diffusivity, and volumic heat capacity calculated at 298.15 K versus the velocity of sound[14−19] together with those of *n*-alkanes and isopentane.[3] The velocity of sound values are revised to those at 298.15 K.

other isomers). Actually, the values of the thermal conductivity and thermal diffusivity for 3-ethylpentane and 3-methylheptane are consistent within their groups, as shown in Figure 6. The present result is expected to be utilized for estimating or predicting the unknown thermal properties of similar materials.

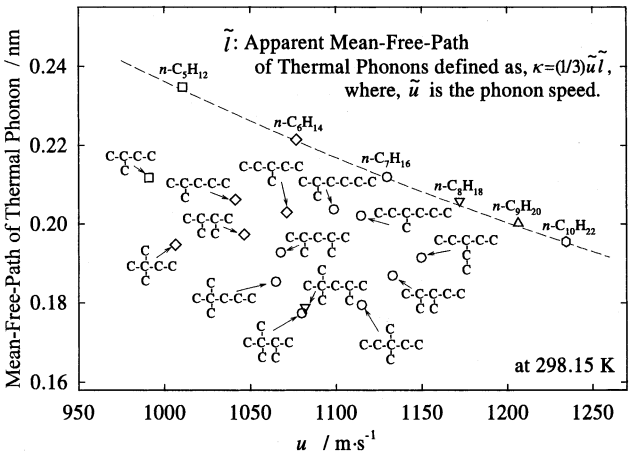

Figure 10. Effectively calculated mean free path of the phonon versus the velocity of sound[14−19] together with those of *n*-alkanes and isopentane.[3]

Acknowledgment

The author thanks Mr. Jose Luis Cravioto Urbina, Engineering and Industrial Development Center, Mexico, for carrying out part of the measurements.

Literature Cited

(1) Watanabe, H. Accurate and simultaneous measurement of the thermal conductivity and thermal diffusivity of liquids using the transient hot-wire method. *Metrologia* **1996**, *33*, 101−115.
(2) Watanabe, H. Further examination of the transient hot-wire method for the simultaneous measurement of thermal conductivity and thermal diffusivity. *Metrologia* **2002**, *39*, 65−81.
(3) Watanabe, H.; Seong, D. J. The Thermal Conductivity and Thermal Diffusivity of Liquid *n*-Alkanes: C_nH_{2n+2} (n=5 to 10) and Toluene. *Int. J. Thermophys.* **2002**, *23*, 337−356.
(4) Watanabe, H.; Cravioto-Urbina, J. L. Measurement of the Thermal Conductivity and Thermal Diffusivity of Isomers of Alkane: C_6H_{14}. *Proc. 20th Jpn. Symp. Thermophys. Prop.* **1999**, 563−566.
(5) Watanabe, H. Accurate and Simultaneous Measurement of the Thermal Conductivity and Thermal Diffusivity of Alkanes: C_7H_{16}. *Proc. 21st Jpn. Symp. Thermophys. Prop.* **2000**, 324−326.
(6) Watanabe, H. Accurate and Simultaneous Measurement of the Thermal Conductivity and Thermal Diffusivity of Some Alkane Isomers: C_nH_{2n+2} (n=7, 8). *Proc. 22nd Jpn. Symp. Thermophys. Prop.* **2001**, 365−367.
(7) *Kagaku Binran II* (Chemical Handbook); Edited by Chem. Soc. Jpn.: Tokyo, Maruzen, 1993; pp II-229−232.
(8) Nagasaka, Y.; Kita, Y.; Nagashima, A. Thermal Conductivity of Liquid Paraffin Hydrocarbons. *Proc. 6th Jpn. Symp. Thermophys. Prop.* **1985**, 49−52.
(9) *TRC Thermodynamic Tables, Hydrocarbons. Vol. I & Vol. X*; Thermodynamic Research Center, The Texas A&M University System: College Station, TX, 1992.
(10) Weber, H. F. *Wiedermann's Ann., Phys. Chem.* **1880**, *10*, 103 (original not seen).
(11) Kuong, J. F. Thermal Conductivity of Liquids. *Br. Chem. Eng.* **1963**, *8*, 356.
(12) Robbins, L. A.; Kingrea, C. L. Estimate Thermal Conductivity. *Hydrocarbon Process. Pet. Refin.* **1962**, *41*, 133−136.
(13) Watanabe, H. To be presented in *Proc. 23rd Jpn. Symp. Thermophys. Prop.*
(14) Schaafs, W. Molecular Acoustics. (2.1.2 Sound-velocity-in-liquids). In *Landolt-Börnstein, New Series, Group II, Vol. 5*; Hellwege, K.-H., Ed.; Springer-Verlag: Berlin, 1967.
(15) Tardajos, G.; Diaz-Peña, M.; Aicart, E. Speed of Sound in Pure liquids by a Pulse-echo-overlap Method. *J. Chem. Thermodyn.* **1986**, *18*, 683−689.
(16) Awwad, A. M.; North, A. M.; Pethrick, R. A. Packing and Conformational Contribution in Binary Liquid Mixtures. *J. Chem. Soc., Faraday Trans.* **1983**, *79*, 2333−2341.
(17) Tamura, K.; Kumaran, M. K.; Halpin, C. J.; Benson, G. C. Ultrasonic speeds and isentropic Compressibilities of Each of the Mixtures: (2-Ethylbutan-1-ol+an Isomer of Hexane) at 298.15 K. *J. Chem. Thermodyn.* **1984**, *16*, 145−152.
(18) Nath, J. Speed of Sound in and Isentropic Compressibilities of (*n*-Butanol+*n*-Pentane, or *n*-Hexane, or *n*-Heptane, or *n*-Octane, or 2,2,4-Trimethylpentane, or Carbon Tetrachloride) at T=293.15 K. *J. Chem. Thermodyn.* **1997**, *29*, 853−863.
(19) Nath, J. Speed of Sound in and Isentropic Compressibilities of (*n*-Butanol+*n*-Pentane) at T=298.15 K, and (*n*-Butanol+*n*-Hexane, or *n*-Heptane, or *n*-Octane, or 2,2,4-Trimethylpentane) at T=303.15 K. *J. Chem. Thermodyn.* **1998**, *30*, 885−895.
(20) Watanabe, H.; Iizuka, K. The Influence of Dissolved Gases on Density of Water. *Metrologia* **1985**, *21*, 19−26.

Received for review July 4, 2002. Accepted September 17, 2002.

JE020125E