Ideal Gas Thermodynamic Properties of Ethane and Propane

J. Chao, R. C. Wilhoit, and B. J. Zwolinski

Thermodynamics Research Center, Texas A&M University, College Station, Texas 77843

The thermodynamic properties (C_p°, S°, H°–H_0°, $(H^\circ$–$H_0^\circ)/T$, $-(G^\circ$–$H_0^\circ)/T$, ΔHf°, ΔGf° and log Kf) for ethane and propane in the ideal gaseous state in the temperature range from 0 to 1500 K and at 1 atm were calculated by statistical thermodynamic methods based on a rigid-rotor harmonic-oscillator model. The internal rotation contributions to thermodynamic functions were evaluated by using a partition function formed by summation of internal rotation energy levels. The calculated heat capacities and entropies compare favorably with available experimental data.

Key words: Critically evaluated data; enthalpy; enthalpy function; enthalpy of formation; entropy; equilibrium constant of formation; ethane; Gibbs energy function; Gibbs energy of formation; heat capacity; ideal gas thermodynamic properties; internal rotation; internal rotation barrier height; internal rotation energy levels; propane; torsional frequencies.

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1. Introduction

Ethane and propane are two basic organic raw materials used extensively in chemical and petrochemical industries for manufacture of numerous important products. The thermodynamic properties for these two compounds have been investigated intensively by many researchers over a long period. In view of the availability of more reliable molecular and spectroscopic constants and of changes in the fundamental constants [1][1], the ideal gas chemical thermodynamic properties for ethane and propane have been re-evaluated in the temperature range from 0 to 1500 K and at 1 atm. The mass units used are C = 12.011 and H = 1.008 (1969 atomic weights).

The contribution of internal rotation of the methyl groups to the thermodynamic properties of ethane and propane was calculated by use of partition functions formed by summation of the internal rotation energy levels for each CH_3 rotor. These energy levels were generated using a procedure developed by Laane, et al. [32]. The calculated internal rotational contributions to thermodynamic properties were added to the contributions from the other degrees of freedom, less internal rotation of each methyl group, to yield the thermodynamic properties as shown in tables 6 and 15.[2]

The calculated heat capacities and entropies are compared with the available measured values in tables 8 and 16.

2. Ethane

Ethane (C_2H_6) has been a subject of great interest to chemists and physicists for many years. Since the work of Kemp and Pitzer [2, 3] established the existence of a potential barrier hindering the free rotation of the CH_3 group about the C–C bond in the CH_3CH_3 molecule, a significant number of experimental as well as theoretical investigations have been devoted to the study of the

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[1] Figures in brackets indicate literature references in section 6.

[2] All tables have been placed at the end of this paper.

molecular properties of ethane. These molecular data are needed for the calculation of the thermodynamic properties of ethane in the ideal gaseous state by statistical thermodynamic techniques. The method of selection of these values for calculation is described as follows.

The structural parameters of the ethane molecule have been elucidated from electron diffraction studies [4, 5], and infrared [6, 7] and Raman [8, 9] spectra. Because of its high symmetry (D_{3d}), ethane has no permanent dipole moment and hence cannot be studied by microwave techniques. Four sets of typical results obtained by use of different experimental methods are presented in table 1. The values determined by Shaw, Lepard, and Welsh [9] from the rotational constants derived from the Raman spectrum were adopted for this work. Based on these data, we derived the three principal moments of inertia as: $I_A = 10.4811 \times 10^{-40}$ and $I_B = I_C = 42.2486 \times 10^{-40}$ g cm^2. The product $I_A I_B I_C$ was 1.8708×10^{-116} g^3 cm^6 and the reduced moment (I_r) for internal rotation was calculated to be 2.6203×10^{-40} g cm^2.

The vibrational frequencies of ethane have been investigated extensively by analyses of infrared [6, 7, 10–16] and Raman [8, 17–20] spectra. Recently, Shimanouchi [21] has reviewed the reported spectral data on ethane and selected a complete set of vibrational wavenumbers for this molecule as shown in table 2 (units in cm^{-1}).[3] In the same table two important sets of vibrational assignments reported in the literature are listed. The values given by Smith [10] were evaluated from the infrared spectrum and those by Lepard, Shaw, and Welsh [19] were obtained from the Raman spectrum.

The hindered internal rotation of the two methyl groups in ethane has been a subject of intensive research since the 1930's. Because the torsional vibration is inactive in both the infrared and Raman spectra of ethane, spectroscopists were forced to deduce the torsional frequency (ν_4) from combination bands. Most determinations favor a value near 290 cm^{-1} as shown in table 3. Based on low temperature heat capacity data, Wilson [29] and Kistiakowsky, et al. [26] derived ν_4 as 280 and 275 cm^{-1}, respectively. Lambert and Salter [30] analyzed the ultrasonic relaxation data on ethane and evaluated the torsional vibration wavenumber to be 290 cm^{-1} Recently, the direct excitation of the torsional vibration in ethane was observed in a slow-neutron inelastic-scattering experiment by Strong and Brugger [31]. Theoretical curves fitted by them to the data indicated that the frequency of transition from the zero to first excited state of this oscillation was 277 cm^{-1}, and a barrier height of 2.75 kcal mol^{-1} was derived. It is known that selection rules often break down as the result of intermolecular interactions or interaction among vibrations causing forbidden transitions to become possible. Based on this fact Weiss and Leroi [15] recorded the infrared spectrum of ethane in the region of the torsional fundamental and first overtone under high-pressure-path-length conditions. This was the first time that the torsional spectra of gaseous ethane have been observed directly in the infrared. The fundmental, ν_4 ($0 \rightarrow 1$), was observed at 289 cm^{-1}. From the above results, as listed in table 3, we adopted the value 289 cm^{-1}, which was observed directly in the infrared by Weiss and Leroi [15], as the torsional wavenumber ν_4 for ethane for our calculation of the internal rotation contributions to thermodynamic properties.

Table 4 summarizes the reported potential barriers to internal rotation in ethane in the period 1932–1970. Except for the values of Eyring [28], Howard [27] and R. M. Pitzer [23], the barrier heights reported by the remaining investigators are in reasonable agreement. It should be emphasized that those reported V_0's were derived based on different molecular structures (see table 1). Therefore direct comparison of the listed values is not appropriate, strictly speaking. Using the adopted $\nu_4 = 289$ cm^{-1}, we calculated $V_0 = 2.96$ kcal mol^{-1} for ethane.

By use of the selected molecular data, as shown in table 5, the ideal gas thermodynamic functions $(H^\circ - H^\circ_0)$, $-(G^\circ - H^\circ_0)/T$, $(H^\circ - H^\circ_0)/T$, S°, and C°_p) for ethane in the temperature range 50–1500 K were evaluated by the statistical thermodynamic method based on a rigid-rotor harmonic-oscillator model. The internal rotation contributions to thermodynamic properties were calculated separately by using the internal rotation partition function obtained by summation of 87 energy levels (0 to 20120 cm^{-1}) derived from the adopted potential function $V = \frac{1}{2} V_0 (1 - \cos 3\theta)$ where $V_0 = 2.96$ kcal mol^{-1} and $\theta =$ angle of internal rotation [32]. The calculated first three energy levels (289, 545, and 549 cm^{-1}) are in agreement with observed peaks (289, 544, and 547 cm^{-1}) reported by Weiss and Leroi [15]. The values thus obtained were added to the contribution from other degrees of freedom (i.e. translation, rotation, vibration, and electronic) less internal rotation. The results are presented in table 6.

Based on the thermodynamic functions $(H^\circ - H^\circ_0)$ and $-(G^\circ - H^\circ_0)/T$ for C (c) and H_2 (g) from [33], for C_2H_6 (g) from this study, and ΔHf° (298.15, C_2H_6, g) $= -20.24$ kcal mol^{-1} [34], the values of ΔHf°, ΔGf° and log Kf in the temperatures 50–1500 K were derived and given in table 6.

3. Propane

Propane (C_3H_8) is the simplest hydrocarbon which has more than one methyl internal rotation in the molecule. Investigations on the internal rotation problem in propane have been pursued by chemists for decades. The solution of this problem may lead to a better understanding of internal rotations in more complex organic

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[3] In keeping with the common convention in molecular spectroscopy, the fundamental frequencies and vibrational energies are frequently expressed in their wavenumber (cm^{-1}) equivalents. The actual frequency in units of hertz may be obtained by multiplying the numbers in these tables by the speed of light expressed in centimeters per second. Energies are obtained by multiplying the frequencies by Planck's constant.

molecules. The research work on the determination of the torsional frequency and potential barrier to internal rotation of the two methyl groups in propane is briefly reviewed in this report. The thermodynamic properties of propane were evaluated by using the most recent molecular data. The procedures employed for the selection of the molecular constants and calculation of the functions are described as follows.

The molecular structure of propane has been investigated by electron diffraction [47,48] and microwave spectroscopy [49]. The molecular parameters obtained from these investigations are summarized in table 9. The values given by Lide [49] were adopted for calculation of the reduced moment (I_r) for internal rotation of the CH_3 group in propane as 4.4202×10^{-40} g cm^2. For the reduced moment calculation, the internal rotations of the two CH_3 rotors were assumed to be independent of each other. The product of the three principal moments of inertia was calculated from the ground-state rotational constants of reference [49].

The infrared spectrum of propane has been observed extensively by many researchers [50–58]. Bartholome [50], Kohlrausch and Köppl [59], and Elyaschevich and Stepanov [51] have studied the Raman spectra of propane. By use of theoretical calculation, Takahashi [60], Schachtschneider and Snyder [61], Gayles, et al. [62], and Shimanouchi [21] assigned different vibrational wavenumbers for propane. Based on their excellent infrared absorption spectrum, Wu and Barker [57] made the most detailed assignment at that time. Later, Pitzer [63] extended their assignment and reported definite values (within 2%) for all frequencies in good agreement with spectral information and thermodynamic data for propane. The fundamental frequencies are listed in table 10 together with three other sets of vibrational assignments. The assignments by Schachtschneider and Snyder [61] were based on extensive normal coordinate calculations on the extended n-paraffins C_2H_6 through n-$C_{14}H_{30}$ and polyethylene, using a perturbation method which adjusted force constants for any number of molecules simultaneously. Gayles, et al. [62] assigned their vibrational wavenumbers based upon the observed band types and rotational structure, frequency shifts upon deuterium substitution, published assignments for the propanes and previous work on the characteristic normal modes of the methyl group [71, 72]. Recently, Shimanouchi [21] critically reviewed the reported spectra data and assigned a complete set of vibrational wavenumbers (see table 10). His reported values were adopted for evaluation of the thermodynamic properties for propane, except for the two torsional wavenumbers, ν_{14} and ν_{27}.

The two torsional frequencies in propane have been directly measured at 217 ± 8 and 265 ± 8 cm^{-1} recently by Grant, et al. [74] with inelastically scattered neutrons using the "small k" method of neutron molecular spectroscopy (NMS). Not subject to the same selection rules as optical spectroscopy, NMS is capable of observing vibrational transitions which are otherwise forbidden by molecular symmetry. The vibrational frequencies were interpreted by numerically solving the wave equation based upon a two-dimensional Fourier expansion of the potential energy. They obtained a $V_3=3680 \pm 190$ cal mol^{-1} for individual methyl-group librations and a $V_6=-280 \pm 130$ cal mol^{-1} term which couples the two methyl tops. The microwave spectrum of propane in the ground torsional state has been observed by Lide [49], and he did not observe any splitting due to internal rotation. He concluded that the barrier height for internal rotation of a methyl group must be at least 2700 cal mol^{-1}. This value is consistent with the other reported V_3 barriers, as presented in table 12. Hirota, *et al.* [64] observed the microwave spectrum of propane in the first-excited states of the CH_3 torsion. The top-top interaction and its effect on the rotational spectra were treated by perturbation theory. They reported that the rotational barrier is described by a threefold parameter $V_3=3325 \pm 20$ cal mol^{-1} and a coupling parameter $V_6=-170 \pm 20$ cal mol^{-1}. The two methyl torsional frequencies were calculated as 216.1 and 270.7 cm^{-1}.

Hoyland [65] reanalyzed the data of Hirota, et al. [64] and carried out quantum-mechanical calculations on various conformations of the propane molecule using a Gaussian basis set and the Hartree-Fock-Roothaan Formalism. He obtained $V_3=3575 \pm 100$ cal mol^{-1} and a coupling term $V_6=-310 \pm 40$ cal mol^{-1}. These values imply $\nu_{14}=216.2$ and $\nu_{27}=268.1$ cm^{-1}. By the high-pressure-long-path-length technique, Weiss and Leroi observed a weak peak at 264 cm^{-1}, which they assigned to the B_2 torsional frequency, and determined $V_3=2945$ and $V_6=-283$ cal mol^{-1} [74]. The reported methyl torsional frequencies and internal rotation potential barrier in propane are summarized in tables 11 and 12.

Using their values for the A_2 and B_2 torsional modes, Grant, et al. [74] obtained the first five propane torsional energy levels as: 0, 217.1, 265.5, 431.1, 465.5, and 523.7 cm^{-1}. The higher energy states were not calculated because of the unknown tunneling which will perturb the higher states. Evaluation of additional Fourier constants in the potential-energy expansion must await additional spectroscopic data concerning higher vibrational levels. Since we cannot now obtain the complete set of propane torsional energy levels derived from the two-dimensional potential function including the coupling effect of the two methyl tops, the partition function was calculated on the assumption of two independent one-dimensional internal rotations with identical barrier heights.

The thermodynamic properties of propane listed in table 15 were calculated from the selected molecular parameters given in tables 10, 11, 12, and 14 for the rigid-rotor harmonic-oscillator model. The partition function for internal rotation was calculated from two identical sets of 113 levels from 0 to 20300 cm^{-1} generated from a computer solution of the Schroedinger equation [32].

The values of ΔHf°, ΔGf° and $\log Kf$ in the temperature range from 0 to 1500 K were derived using $(H^{\circ}-H_0^{\circ})$ and $-(G^{\circ}-H_0^{\circ})/T$ for C (c) and H_2 (g) from [33], for C_3H_8 (g) from this work, and ΔHf° (298.15, C_3H_8,g) $=-24.82$ kcal mol^{-1} from [34]. The results are shown in table 15.

4. Discussion

Ethane is an important raw material used extensively in petrochemical industries for manufacture of various organic chemicals. The low temperature heat capacities (15.5–184.1 K), melting point (89.87±0.1 K), and enthalpies of fusion (682.9±0.7 cal mol^{-1}) and vaporization (3514±3.5 cal mol^{-1}) were measured by Witt and Kemp [35] in 1937. They derived the third law entropy of ethane (g) at the boiling point (184.1±0.1 K) to be 49.38±0.15 cal K^{-1} mol^{-1}. Adopting a correction for gas imperfection as 0.16 cal K^{-1} mol^{-1}, they obtained the entropy of ideal gas at the boiling point as 49.54 cal K^{-1} mol^{-1}. Using a correction for the gas imperfection as 0.19 cal K^{-1} mol^{-1} [34], we recalculated the value of S° (184.1, C_2H_6, g) to be 49.57±0.15 cal K^{-1} mol^{-1}. The S° value obtained by the present statistical thermodynamic calculation is 49.48 cal K^{-1} mol^{-1} which is in agreement with the third law entropy value within the experimental uncertainty.

The heat capacities of ethane (g) in the temperature range 92.4–603.2 K have been determined by many investigators; the most reliable of these studies are listed in table 7. Table 8 compares the selected experimental values with the calculated ones. In consideration of the precision of the experimental equipment available at that time, the agreement between the C_p° values from this work and the measured ones as listed in table 8 are excellent. For consistency, we converted the reported real gas heat capacities for ethane to ideal gas heat capacities by use of the gas imperfection corrections from the API Research Project 44 Tables [34]. It is interesting to note that our gas imperfection corrections for the C_p data of Dailey and Felsing [46] are virtually the same as those used by the authors in 1943. The results in table 8 illustrate the good agreement of our calculated thermodynamic properties for ethane (g) with the available experimental measurements.

Kemp and Egan [67] measured the low temperature heat capacities, 13.29–231.04 K, for propane. They also determined enthalpies of fusion (842.2±0.8 cal mol^{-1}), and vaporization (4487±4 cal mol^{-1}) and the melting (85.45±0.05 K) and boiling (231.04±0.05 K) points. Based on these data they derived the entropies of the real and ideal gas at the boiling point as 60.29±0.1 and 60.45 cal K^{-1} mol^{-1}, respectively. Using the value of the correction for the gas imperfection, 0.21 cal K^{-1} mol^{-1} from API 44 tables [34], instead of 0.16 cal K^{-1} mol^{-1} used by Kemp and Egan, we recalculated the entropy of propane in the ideal gaseous state at 1 atm and 231.04 K to be 60.50±0.12 cal K^{-1} mol^{-1} which is in excellent agreement with our entropy value of 60.50 ±0.1 cal K^{-1} mol^{-1} obtained from statistical thermodynamic calculations. The entropy value calculated by Pitzer [63] was 60.46±0.1 cal K^{-1} mol^{-1}. He also reported the entropy of propane at 180.0 K as 57.04 ± 0.1 cal K^{-1} mol^{-1} while our value is 57.11 cal K^{-1} mol^{-1}.

The heat capacities of propane (g) have been determined by Beeck (273–573 K) [42], Sage, et al. (294–444 K) [73], Kistiakowsky, et al. (148–258 K) [70], Kistiakowsky and Rice (272–369) [69], and Dailey and Felsing (344–693 K) [46]. For consistency, their reported C_p values were converted to those in the ideal gaseous state (C_p°) by using the values of the correction for the gas imperfection obtained from API 44 tables [34]. The results are compared with our calculated values as shown in table 16. The agreement between our values and those measured by Kistiakowsky, et al. [70], Kistiakowsky and Rice [69], and Dailey and Felsing [46] is reasonably good.

The calculated heat capacities and entropies for ethane and propane are compared with those given in the API 44 tables [34] in table 17.

The calculation of all the energy levels associated with the internal rotations of the two methyl groups in propane is still in an unsatisfactory state. In the normal coordinate treatment this torsional motion is described in terms of two symmetry coordinates which account for the two harmonic oscillations identified by ν_{14} and ν_{27} in table 10. The frequencies of these two oscillations, and their corresponding reduced moments of inertia, are different even when it is assumed that there are no cross terms in the potential energy for the internal rotations of the two groups. Grant, et al. [74], and others, have shown, moreover, that the energy levels are significantly perturbed by the effect of interaction terms in the potential energy. An exact set of energy levels is not necessarily required for a reliable statistical calculation of thermodynamic properties since the interactions tend to split levels in a roughly symmetric way. Thus the effect on the partition function will be small as long as the perturbation is much smaller than kT.

Table 13 shows a comparison of heat capacity and entropy calculated from several approximate sets of energy levels for internal rotation. In each case two sets of levels for a single internal rotor whose potential energy is given by the usual three-fold cosine function of rotational angle were used. In the first three lines, two identical sets, corresponding to the fundamental frequency listed, were used. The value of 210 cm^{-1} is the average of ν_{14} and ν_{27} obtained by Schachtschneider and Snyder [61] while 241 cm^{-1} is the average of the two values reported by Grant, et al. [74]. The results for 241 cm^{-1} agree better with the experimental heat capacity and entropy than do those for 210 cm^{-1}. The results obtained when two different sets of levels, corresponding to the ν_{14} and ν_{27} of Grant, et al., were used are given in the fourth line. These do not differ from the third line by an experimentally significant amount. An additional series of calculations of thermodynamic properties in the range from 50 to 200 K was also made with about 12 internal rotational levels. Higher levels do not contribute at these temperatures. These sets of levels were obtained by combining the first five levels of Grant, et al., with higher levels approximated in various ways, including those corresponding to table 13. No significant differences were obtained in the results. Hirota, et al. [64] tried to neglect the top-top coupling and calculated the $\nu(0 \rightarrow 1)$ transition as 243.4 cm^{-1} and $V_0 = 3.325$ kcal mol^{-1} which are in reasonable agreement with our selected values.

5. Acknowledgment

This study was partially supported by the American Petroleum Institute Research Project 44 of the Thermodynamics Research Center and the Texas Engineering Experiment Station of Texas A&M University.

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TABLE 1. Structural data for ethane

Structural parameter[a]	Reference			
	Almenningen and Bastiansen (1955)[b]	Allen and Plyler (1959)[c]	Lepard, et al. (1962)[d]	Shaw, et al. (1965)[e]
r(C–H)	1.107	(1.093)[f]	1.0914±0.0003	1.095±0.002
r(C–C)	1.536	1.534	1.5362±0.0005	1.534±0.002
∡HCH	109.3°	109.75	108.01±0.06	107.8±0.2

[a] Bond distances, 10^{-8} cm; bond angle, degrees.
[b] Reference [5]; electron diffraction method.
[c] Reference [7]; infrared spectrum.
[d] Reference [8]; Raman spectrum.
[e] Reference [9]; Raman spectrum. These values were adopted.
[f] Estimated value.

TABLE 2. Vibrational assignments for ethane (cm^{-1})

Mode no.	Symmetry species	Reference		
		Smith (1949)[b]	Lepard, et al. (1966)[c]	Shimanouchi (1972)[a, d]
ν_1	a_{1g}	2955.1 (b) 2899.2 (a)	2953.7	2954
ν_2	a_{1g}	1375	1388.4	1388
ν_3	a_{1g}	993	994.8	995
ν_4	a_{1u}	290	289	289
ν_5	a_{2u}	2954 (b) 2895.7 (a)	2895.8	2896
ν_6	a_{2u}	1379.14	1379.19	1379
ν_7	e_u	2995.5	2995.5	2969
ν_8	e_u	1472.2	1472.2	1468
ν_9	e_u	821.52	821.60	1190
ν_{10}	e_g	2963 (b) 2939.5 (a)	2968.69	2985
ν_{11}	e_g	1460	1468.1	1469
ν_{12}	e_g	1190	1190	822

[a] The reported values were adopted in this work.
[b] Reference [10].
[c] Reference [19].
[d] Reference [21].

TABLE 3. Determinations of the torsional frequency (ν_4) in ethane[a]

Experimental method	ν_4, cm^{-1}	Reference
Combination bands:		
Infrared	290	[10]
	290	[24]
Raman	289	[19]
	278.4	[17]
Low-temperature C_p measurements	280	[29]
	275	[26]
Ultrasonic relaxation data	290	[30]
Slow-neutron inelastic scattering	277±8	[31]
Infrared spectrum	289	[15]

[a] This work adopted the value 289 cm^{-1} for the torsional wavenumber ν_4.

TABLE 4. Reported potential barriers to internal rotation in ethane[a]

V_0, kcal mol^{-1}	Investigator (year)	Reference
2.96	Durig, et al. (1970)	[22]
2.928±0.025	Weiss and Leroi (1968)	[15]
3.5	R. M. Pitzer (1967)	[23][b]
3.03	D. R. Lide (1958)	[24]
2.875±0.125	K. S. Pitzer (1951)	[25]
2.75	Kistiakowsky, et al. (1939)	[26]
3.00	E. B. Wilson (1938)	[29]
3.15	Kemp and Pitzer (1937)	[2]
$\geqslant$ 2.00	J. B. Howard (1937)	[27]
0.36	H. Eyring (1932)	[28]

[a] This work derived $V_0 = 2.96$ kcal mol^{-1} based on the adopted value of torsional frequency $= 289\ \mathrm{cm}^{-1}$.
[b] The reported value was theoretically calculated. In this paper a summary of other theoretically calculated V_0 values is given and references quoted therein.

TABLE 5. Molecular constants for ethane

Molecular weight	30.070
Point group	D_{3d}
Symmetry number	18
Ground state configuration	$^1A_{1g}$
Product of the three principal moments of inertia, g³ cm⁶	1.8708×10^{-116}
Reduced moment, g cm²	2.6203×10^{-40}
Potential barrier height, kcal mol⁻¹	2.96
Vibrational wavenumbers, cm⁻¹	2954, 1388, 995, 2896, 1379, 2969 (2), 1468 (2), 1190 (2), 2985 (2), 1469 (2), 822 (2)

TABLE 6. Ideal gas thermodynamic properties for ethane

T	H°-H°_0	$-\frac{(G^\circ-H^\circ_0)}{T}$	$\frac{(H^\circ-H^\circ_0)}{T}$	S°	C°_p	ΔHf°	ΔGf°	log Kf
K	cal mol⁻¹	cal K⁻¹ mol⁻¹				kcal mol⁻¹		
0	0	0	0	0	0	−16.50	−16.50	infinite
50	398	30.32	7.953	38.27	7.98	−17.62	−16.40	71.68
100	808	35.86	8.082	43.94	8.52	−18.00	−15.04	32.86
150	1252	39.19	8.348	47.53	9.24	−18.48	−13.45	19.60
200	1735	41.63	8.673	50.31	10.10	−19.04	−11.69	12.78
273.15	2534	44.42	9.276	53.70	11.84	−19.94	−8.88	7.10
298.15	2838	45.24	9.520	54.76	12.54	−20.24[a]	−7.84	5.74
300	2862	45.30	9.538	54.84	12.60	−20.26	−7.76	5.65
400	4272	48.20	10.681	58.88	15.65	−21.43	−3.41	1.86
500	5989	50.72	11.978	62.70	18.64	−22.45	1.22	−0.53
600	7990	53.02	13.317	66.34	21.33	−23.30	6.03	−2.20
700	10245	55.17	14.635	69.81	23.71	−24.00	10.98	−3.43
800	12723	57.21	15.903	73.11	25.81	−24.56	16.01	−4.38
900	15398	59.15	17.109	76.26	27.67	−24.99	21.11	−5.13
1000	18249	61.02	18.249	79.26	29.30	−25.30	26.26	−5.74
1100	21252	62.81	19.320	82.13	30.73	−25.52	31.40	−6.24
1200	24390	64.53	20.325	84.86	31.99	−25.66	36.61	−6.67
1300	27644	66.20	21.265	87.46	33.08	−25.75	41.80	−7.03
1400	31002	67.80	22.144	89.95	34.04	−25.78	47.02	−7.34
1500	34449	69.36	22.966	92.33	34.87	−25.77	52.20	−7.61

1 cal = 4.184 J

[a] While this paper was in proof, Pittam and Pilcher reported a new value of −20.04 kcal mol⁻¹ for ΔHf°(g, 298.15 K) ethane. J. Chem. Soc. Faraday Trans. I **68**, 2224 (1972).

TABLE 7. Summary of heat capacity measurements for ethane

Investigator	Number of data points	Temperature, K	Reference
Scheel and Heuse (1913)	3	191.2–288.2	[36]
Heuse (1919)	3	191.2–288.2	[37]
Partington and Shilling (1924)	3	283.2–373.2	[38]
Thayer and Stegeman (1931)	4	275.4–337.6	[39]
Eucken and Parts (1933)	7	189.1–373.5	[40]
Eucken and Weigert (1933)	5	143 –280	[41]
Beeck (1936)	4	273.2–573.2	[42]
Kistiakowsky and Nazmi (1938)	2	143 –163	[43]
Kistiakowsky, et al. (1939)	9	92.4–134.1	[44]
Kistiakowsky and Rice (1939)	4	272.1–364.8	[45]
Dailey and Felsing (1943)	7	347.7–603.2	[46]

TABLE 8. Comparison of calculated and measured heat capacities for ethane[a]

T	C_p	C_p-C_p°	C_p°		C_p° (calc.)-
K			Experimental	Calculated	C_p° (exptl.)
			Dailey and Felsing (1943)		
347.7	14.14	0.07	14.07	14.03	−0.04
359.8	14.49	0.06	14.43	14.40	−0.03
387.6	15.32	0.05	15.27	15.27	0.00
452.0	17.34	0.03	17.31	17.24	−0.07
520.6	19.16	0.02	19.14	19.22	+0.08
561.6	20.64	0.01	20.63	20.33	−0.30
603.2	21.63	0.01	21.62	21.41	−0.21
			Kistiakowsky and Rice (1939)		
272.07	11.96	0.17	11.79	11.81	+0.02
302.70	12.82	0.12	12.70	12.67	−0.03
335.82	13.79	0.08	13.71	13.67	−0.04
364.78	14.64	0.06	14.58	14.56	−0.02
			Eucken and Parts (1933)		
189.2	10.48	0.61	9.87	9.89	+0.02
209.3	10.68	0.46	10.22	10.29	+0.07
229.6	11.02	0.31	10.71	10.74	+0.03
249.9	11.48	0.23	11.25	11.23	−0.02
250.2	11.46	0.23	11.23	11.23	0.00
272.0	12.01	0.17	11.84	11.81	−0.03
292.0	12.57	0.16	12.41	12.36	−0.05
373.6	14.90	0.05	14.85	14.83	−0.02
			Heuse (1919)		
191.2	10.44	0.60	9.84	9.93	+0.09
238.2	11.04	0.27	10.77	10.94	+0.17
288.2	12.40	0.13	12.27	12.26	−0.01

[a] Unit = cal K^{-1} mol^{-1}; 1 cal = 4.184 J.

TABLE 9. Structural data for propane

Structural parameter[a]	Reference		
	Wierl (1932)[b]	Bauer (1936)[c]	Lide (1960)[d]
r(C–C)	1.52 ± 0.05	1.50 ± 0.02	1.526 ± 0.002
∡ CCC	(109.47)[e]	114	112.4 ± 0.2
r(C–H), in CH_2	1.10	1.08 ± 0.02	1.096 ± 0.002
∡ HCH, in CH_2	(109.47)		106.1 ± 0.2
r(C–H), in CH_3	1.10		1.091 ± 0.01
∡ HCH, in CH_3	(109.47)		107.7 ± 1.0

[a] *Bond distances*, 10^{-8} cm; bond angle, degrees.

[b] Reference [47].

[c] Reference [48].

[d] Reference [49]; the reported values were adopted in this work.

[e] Estimated value.

TABLE 10. Vibrational assignments for propane (cm^{-1})

Mode no.	Symmetry species	Reference				
		Wu and Barker (1941)[a]	Pitzer (1944)[b]	Schachtschneider and Snyder (1963)[c]	Gayles and King (1965)[d]	Schimanouchi (1972)[e]
ν_1	a_1	2966	2966	2966	2976.7	2977
ν_2	a_1	2960	2960	2882	2961.7	2962
ν_3	a_1	2914	2914	2856	2887.0	2887
ν_4	a_1	1436	1460	1471	1476.0	1476
ν_5	a_1	1468	1468	1445	1462.0	1462
ν_6	a_1	1370	1370	1378	1391.9	1392
ν_7	a_1	1149	1155	1151	1157.5	1158
ν_8	a_1	867	868	870	869.3	869
ν_9	a_1	375	375	382	369.2	369
ν_{10}	a_2		2970	2964		2967
ν_{11}	a_2	1436	1450	1459		1451
ν_{12}	a_2	1361	1278	1279	(1292)	1278
ν_{13}	a_2	870	940	903		940
ν_{14}	a_2		(202)	200	(208)	216
ν_{15}	b_1	2968	2968	2963	2968.2	2968
ν_{16}	b_1	2942	2942	2882	2887.0	2887
ν_{17}	b_1	1465	1470	1465	1464.0	1464
ν_{18}	b_1	1375	1375	1367	1378.0	1378
ν_{19}	b_1		1338	1342	1338.4	1338
ν_{20}	b_1	1053	1053	1046	1053.8	1054
ν_{21}	b_1	922	922	924	921.7	922
ν_{22}	b_2	2980	2980	2965	2972.6	2973
ν_{23}	b_2	2968	2968	2921	2968.2	2968
ν_{24}	b_2	1443	1450	1464	1472.0	1472
ν_{25}	b_2	1179	1179	1185	1191.5	1192
ν_{26}	b_2	748	748	747	748.1	748
ν_{27}	b_2		(283)	220	(223.0)	268

[a] Reference [57].

[b] Reference [63].

[c] Reference [61].

[d] Reference [58].

[e] Reference [21], the reported values adopted in this work except ν_{14} and ν_{27}.

TABLE 11. Summary of reported torsional frequencies in propane

Torsional frequency, cm^{-1}		Method of determination	Reference
ν_{14}	ν_{27}		
202	283	calculated	[63]
200	220	calculated	[61]
208	223	estimated from combination band	[58]
202	225	calculated	[62]
216.1	270.7	calculated	[64]
243	243	calculated	
216.2	268.1	calculated	[65]
217±8	265 ± 8	directly measured	[74]
	264[a]		
216	268	calculated	[21]
241	241	selected by this work	

[a] This transition was observed by Weiss and Leroi; quoted by Grant, et al. [74] as private communication.

TABLE 12. Reported potential barriers to internal rotation in propane

V_3	V_6	Investigator (year)	Reference
kcal mol^{-1}			
3.40		Pitzer (1937)	[66]
3.30		Kemp and Egan (1938)	[67]
3.40		Pitzer (1940)	[68]
3.1 – 3.2		Kistiakowsky and Rice (1940)	[69]
3.30		Kistiakowsky, et al. (1940)	[70]
3.40		Pitzer (1944)	[63]
3.40		Pitzer (1951)	[25]
>2.70		Lide (1960)	[49]
3.325	−0.170	Hirota, et al. (1967)	[64]
3.575	−0.310	Hoyland (1968)	[65]
3.33		Durig, et al. (1970)	[22]
3.680	−0.280	Grant, et al. (1970)	[74]
2.945	−0.283	Weiss and Leroi[a]	
3.29		This work	

[a] Quoted by Grant, et al. [74] as private communication.

TABLE 13. Comparison of calculated C_p° and S° for propane[a]

Torsional frequency		Potential barrier	C_p°			S°		
ν_{14}	ν_{27}	V_0	298.15 K	500 K	1000 K	298.15 K	500 K	1000 K
210	210	2.55, 2.55	17.65	26.48	41.38	65.21	76.46	99.94
239	239	3.25, 3.25	17.60	26.89	41.71	64.61	75.96	99.73
241	241	3.29, 3.29	17.59	26.91	41.73	64.58	75.93	99.72
217	265	2.71, 3.94	17.54	26.84	41.75	64.60	75.92	99.70

[a] Units: cm^{-1} for torsional frequency; kcal mol^{-1} for potential barrier; cal K^{-1} mol^{-1} for C_p° and S°.

TABLE 14. Molecular constants for propane

Molecular weight	44.097
Point group	C_{2V}
Symmetry number	18
Ground state configuration	$^1A_{1g}$
Product of the three principal moments of inertia, $I_AI_BI_C$, g^3 cm^6	3.2148×10^{-115}
Reduced moment, I_r, g cm^2	4.4202×10^{-40}
Potential barrier height, kcal mol^{-1}	3.29
Vibrational wavenumber, cm^{-1}	2977, 2962, 2887, 1476, 1462, 1392, 1158, 869, 369, 2967, 1451, 1278, 940, 2968, 2887, 1464, 1378, 1338, 1054, 922, 2973, 2968, 1472, 1192, 748

TABLE 15. Ideal gas thermodynamic properties for propane (g)

T	$H^\circ - H_0^\circ$	$-\frac{(G^\circ - H_0^\circ)}{T}$	$\frac{(H^\circ - H_0^\circ)}{T}$	S°	C_p°	ΔHf°	ΔGf°	log Kf
K	cal mol^{-1}	cal K^{-1} mol^{-1}				kcal mol^{-1}		
0	0	0	0	0	0	−19.50	−19.50	infinite
50	399	36.44	7.976	44.42	8.14	−21.11	−19.15	83.72
100	845	42.09	8.453	50.54	9.87	−21.73	−16.96	37.07
150	1385	45.66	9.231	54.89	11.66	−22.42	−14.43	21.02
200	2011	48.43	10.053	58.48	13.40	−23.21	−11.64	12.72
273.15	3098	51.75	11.341	63.09	16.43	−24.42	−7.24	5.79
298.15	3523	52.76	11.816	64.58	17.59	−24.82[a]	−5.63	4.13
300	3555	52.83	11.852	64.68	17.67	−24.85	−5.51	4.01
400	5563	56.52	13.907	70.43	22.47	−26.36	1.18	−0.64
500	8036	59.85	16.072	75.93	26.91	−27.64	8.21	−3.59
600	10924	62.97	18.207	81.18	30.76	−28.68	15.48	−5.64
700	14171	65.94	20.245	86.18	34.10	−29.52	22.91	−7.15
800	17729	68.77	22.161	90.93	36.99	−30.16	30.45	−8.32
900	21558	71.48	23.953	95.43	39.52	−30.64	38.05	−9.24
1000	25623	74.09	25.623	99.72	41.73	−30.96	45.72	−9.99
1100	29895	76.61	27.178	103.79	43.66	−31.15	53.36	−10.60
1200	34348	79.04	28.623	107.66	45.35	−31.26	61.08	−11.12
1300	38958	81.38	29.967	111.35	46.81	−31.28	68.77	−11.56
1400	43704	83.65	31.217	114.86	48.09	−31.24	76.50	−11.94
1500	48570	85.84	32.380	118.22	49.21	−31.14	84.17	−12.26

1 cal = 4.184 J.

[a] While this paper was in proof, Pittam and Pilcher reported a new value of −25.02 kcal mol^{-1} for ΔHf°(g, 298.15 K) propane. J. Chem. Soc. Faraday Trans. I **68**, 2224 (1972).

TABLE 16. Comparison of calculated and measured heat capacities for propane (g)[a]

T K	C_p	$C_p-C_p^\circ$	C_p° Experimental	C_p° Calculated	C_p° (calc.)−C_p° (exptl.)
O. Beeck (1936)					
273.15	15.86	0.415	15.44	16.43	+0.99
373.15	20.26	0.125	20.14	21.19	+1.05
473.15	24.74	0.055	24.68	25.77	+1.09
573.15	28.71	0.026	28.68	29.78	+1.10
B. H. Sage, D. C. Webster and W. N. Lacey (1937)					
294.3	17.83	0.31	17.52	17.41	−0.11
310.9	18.31	0.25	18.06	18.19	+0.13
327.6	18.79	0.21	18.58	18.99	+0.41
344.3	19.28	0.17	19.11	19.80	+0.69
360.9	19.80	0.14	19.66	20.60	+0.94
377.6	20.32	0.12	20.20	21.40	+1.20
394.3	20.84	0.11	20.73	22.20	+1.47
410.9	21.36	0.09	21.27	22.98	+1.71
427.6	21.88	0.08	21.80	23.75	+1.95
444.3	22.40	0.06	22.34	24.50	+2.16
G. G. Kistiakowsky, J. R. Lacher and W. W. Ransom (1940)					
148.2			11.69	11.60	−0.09
157.8			12.04	11.93	−0.11
213.1			14.00	13.90	−0.10
219.0			14.17	14.13	−0.04
258.0			15.75	15.75	0.00
G. B. Kistiakowsky and W. W. Rice (1940)					
272.38	16.39	0.42	15.97	16.39	+0.42
300.37	17.73	0.25	17.48	17.69	+0.21
334.05	19.35	0.19	19.16	19.30	+0.14
368.55	20.97	0.13	20.84	20.97	+0.13
B. P. Dailey and W. A. Felsing (1943)					
343.7	19.80	0.17	19.63	19.77	+0.14
360.1	20.48	0.14	20.34	20.56	+0.22
387.8	21.72	0.11	21.61	21.89	+0.28
452.6	25.13	0.06	25.07	24.87	−0.20
521.0	27.93	0.04	27.89	27.77	−0.12
562.0	29.13	0.03	29.10	29.37	+0.27
603.3	30.78	0.02	30.76	30.88	+0.12
693.2	33.63	0.015	33.62	33.88	+0.26

[a] Unit = cal K^{-1} mol^{-1}; 1 cal = 4.184 J.

TABLE 17. Comparison of calculated and API 44 tables 1952 values of C_p° and S° for ethane and propane[a]

T K	C_p°, cal K^{-1} mol^{-1} This work	API 44 1952 value	Difference	S°, cal K^{-1} mol^{-1} This work	API 44 1952 value	Difference
Ethane						
100	8.52	8.59	−0.07	43.94	43.94	0.00
298.15	12.54	12.58	−0.04	54.76	54.85	−0.09
700	23.71	23.72	−0.01	69.81	69.93	−0.12
1000	29.30	29.33	−0.03	79.26	79.39	−0.13
1500	34.88	34.90	−0.02	92.32	92.46	−0.14
Propane						
100	9.87	9.84	+0.03	50.54	50.52	+0.02
298.15	17.59	17.57	+0.02	64.58	64.51	+0.07
700	34.10	34.20	−0.10	86.18	86.17	+0.01
1000	41.73	41.83	−0.10	99.72	99.77	−0.05
1500	49.21	49.26	−0.05	118.22	118.29	−0.07

[a] Average percentage difference in C_p° for ethane and propane, respectively: 100−700 K: −0.32 percent, −0.01 percent; 700−1500 K: −0.08 percent, −0.20 percent. Average percentage difference in S° for ethane and propane, respectively: 100−700 K: −0.13 percent, +0.06 percent; 700−1500 K: −0.16 percent, −0.05 percent.