

Thermodynamic Properties of Alkenes (Mono-Olefins Larger Than C₄)

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The thermodynamic properties of the mono-olefins with carbon numbers greater than C₄ were reviewed. Properties included critical properties, vapor pressures, densities, second virial coefficients, enthalpies of vaporization, heat capacities, and enthalpies of combustion. Enthalpies of formation for the liquid, gas, and ideal-gas state at 298.15 K were calculated for 47 compounds based on the experimental values. Sufficient experimental information was available to allow the calculation of entropies, enthalpies, and Gibbs energies for the ideal-gas state (over approximately a 100 K range near 250 K to 400 K) for 14 compounds. Comparisons were made with experimental isomerization equilibria, isomerization enthalpies, and group-contribution estimates for enthalpies of formation and entropies. "Gaps" in the available data were identified and recommendations for additional experiments are made. Evidence for errors in several of the original experimental results is presented, and revised values are suggested.

Key words: alkene; critical properties; critically reviewed data; density; enthalpy of formation; enthalpy of vaporization; entropy; Gibbs energy; heat capacity; ideal-gas properties; second virial coefficients; vapor pressure.

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1. Introduction

1.1. Background

Alkenes are major intermediates of many processes within chemical industry. Indeed, alkene polymerization is one of the most profitable. However, the enhanced reactivity due to the presence of the double bond in the alkene also means that its presence can lead to undesired properties. For example, the presence of alkenes can be a major source of instability in middle distillate fuels. A comprehensive knowledge of the thermodynamic and thermophysical properties of alkenes can aid both chemists and chemical engineers in the design of new, efficient processes for their production and use. The existence of a comprehensive and internally consistent set of thermodynamic and thermophysical properties for the alkenes can also aid in the development of new or improved correlations for the estimation of properties for those alkenes for which experimental measurements have not been made.

1.2. Scope

The scope of this review includes all alkenes larger than C_4 for which sufficient experimental information exists for the calculation of the enthalpy of formation or

the entropy for the ideal-gas state. (Combination of these properties provides the Gibbs energy of formation.) The properties reviewed were enthalpies of combustion, heat capacities (only those sufficient to provide condensed-phase entropies), vapor pressures, enthalpies of vaporization, densities, and second virial coefficients. Selected values were used to calculate entropies, enthalpies of formation, and Gibbs energies of formation for the ideal-gas state for a range of temperatures. Comparisons are made with experimental isomerization equilibria, isomerization enthalpies, and group-contribution estimates for enthalpies of formation and entropies for the ideal-gas state. "Gaps" in the available data are identified and recommendations for additional experiments are made.

The emphasis of the compilation is on the derivation of ideal-gas thermodynamic properties from *experimentally* measured quantities. Estimations and extrapolations are used sparingly, and are indicated and documented clearly. Subsequent users of the compilation can derive their own correlations in the knowledge that they are not making a correlation of data that has already been correlated. It is in the best interest of the experimental thermodynamicist to make a clear distinction between measured and estimated values. Otherwise, "correlations of correlations" will continue to appear in the literature.

1.3. Literature Reviewed

A comprehensive search of the literature via Chemical Abstracts since 1930 was completed. Pre-1930 physical-property information on organic compounds is mainly of historic interest. Some pre-1930 references are cited but, no attempt was made to make a comprehensive search of that literature. Secondary sources (90TRC, 90DOM/HEA, 86PED/NAY, 85MAJ/SVO, 84BOU/FRI, 84DOM/EVA, 83CHA/LIN, 70COX/PIL, 69STU/WES, 50TIM) were also abstracted, and the primary sources were obtained when possible. If a secondary source was used for an experimental value, this is indicated in the tables and references.

2. Thermodynamic Properties

2.1. Critical Properties

Accurate critical-property values allow the reliable estimation of many important thermophysical properties through correlations based upon corresponding states. Experimental measurements are rarely made over a temperature range sufficient to preclude the need for estimations and extrapolations. In the present paper corresponding-states methods are used to estimate densities and second and third virial coefficients required for the calculation of enthalpies of vaporization from vapor-pressure data.

2.1.a. Measured Critical Properties

For alkenes larger than C_4 only six critical temperatures, three critical pressures, and one critical density had

been measured before 1991. In 1991 the research group of Teja (91GUD/ROS) published new measurements for a series of alk-1-enes ranging from C₅ to C₁₂. New measurements were also reported recently by Peisheng *et al.* (91PEI/YOU) for pent-1-ene, 3-methylbut-1-ene, and hex-1-ene. The critical properties measured by Peisheng *et al.* for 3-methylbut-1-ene are only the second for a branched alkene, and are the first in forty years since the work of Kiyama *et al.* (51KIY/SUZ) on 2-methylbut-2-ene. (See section 6.1 below.) All measured critical temperatures and pressures are listed with their sources in Table 1. Teja and co-workers (83WOL/KAY,91GUD/ROS) and Peisheng *et al.* (91PEI/YOU) also reported the only critical densities for alkenes larger than C₄; these are discussed below in Sec. 2.3 (Densities).

2.1.b. Estimation of Critical Properties

It is apparent from Table 1 that most of the critical properties for compounds of interest to this work have not been measured. The group-additivity method of Joback (84JOB) was used to estimate the critical temperature and critical pressure, when measured numbers were not available. There are many published methods, which could have been used for the estimation of the critical properties. The method of Joback was selected partially for its lack of ambiguities in application, and because the database of alkene critical properties is so small that there is little basis to determine whether another estimation method is superior.

2.2. Vapor Pressures

2.2.a. Measured Vapor-Pressures

Compounds of interest to this project for which vapor-pressure data are available are listed in Table 2. The references cited in this table are those for data used in the fits of the Cox equation to the measured vapor pressures, as described in the following section (2.2.b). Nearly all of the vapor pressures used in the fits were determined by Rossini and co-workers (50FOR/CAM, 54CAM/ROS, 55CAM/ROS, 56CAM/ROS, 60CAM/ROS) as part of projects for the American Petroleum Institute (API) or by Scott *et al.* (49SCO/WAD, 50SCO/WAD, 55SCO/FIN) at the Thermodynamics Laboratory in Bartlesville, OK. Measurements by Eisen and Orav (70EIS/ORO) were used for the hept-2-enes and hept-3-enes. Measurements by Eisen and co-workers on hept-1-ene (70EIS/ORO) and oct-1-ene (74MIC/ELW) are in good accord with those of Rossini and co-workers, as shown in Appendix 1.

Experimental vapor pressures not used in the fits are compared graphically with values calculated from the fitted equations in Appendix 1. Michelson *et al.* (74MIC/ELW) have determined vapor pressures for several *cis* and *trans* isomers of straight-chain octenes, nonenes, and decenes by ebulliometric methods (5 values between 0.25 and 1 bar; sample purities near 99 mole percent). These

were not included in this review because neither enthalpies of combustion or entropies have been determined for these materials.

2.2.b. Cox-equation Fits to Measured Vapor Pressures

The Cox equation (36COX) in the form:

$$\ln(p/p_c) = \{1 - (T/T_c)\} \exp\{A + B(T/K) + C(T/K)^2\}, \quad (1)$$

was fitted to the measured vapor pressures with fixed p_c and T_c values listed in Table 1. All temperatures for the experimental vapor pressures were converted to ITS-90 prior to the Cox-equation fit. The vapor-pressure fitting procedure has been described (88STE/ARC, 89CHI/NGU). Parameters derived from the fits are given in Table 2. The acentric factors listed in Table 1 were calculated from the results of the fits. The acentric factor is defined as $\{-\lg(p/p_c) - 1\}$, where p is the vapor pressure at $T_r = 0.7$ and p_c is the critical pressure.

Because the uncertainties in p_c and T_c are generally difficult to assess, and because the temperature ranges of the fitted data are short (typically near 50 K), extrapolations of the vapor-pressure results are tenuous. Extrapolations were limited to approximately 50 K for the calculation of enthalpies of vaporization needed for the calculation of the gas-phase properties. Longer extrapolations were employed when necessary for comparison with literature values.

2.3. Densities

2.3.a. Measured Densities

Measured densities for alkenes reviewed in this project are listed in Table 3. With few exceptions the data are within 10 K of 293.15 K. The purities of the materials used in the density determinations were generally low (<99 mole percent) or not reported. The most notable exceptions to this are the measurements made by Rossini and co-workers (50FOR/CAM, 55CAM/ROS, 56CAM/ROS), which were obtained for well-characterized, high-purity samples as part of projects for API. These results were weighted most heavily in the critical-density estimations described in the following section. For the pentenes, Rossini and co-workers reported densities for pent-1-ene only. The density measurements made by the Dow Chemical Co. (75DOW/GOO), which were made on the high-purity samples used in the enthalpy of combustion determinations (79GOO/SMI), were weighted most heavily for the remaining five pentenes. Many references listed in 90TRC were not included in Table 3 because these were found to be for *cis* and *trans* mixtures, rather than for the pure isomers.

2.3.b. Estimation of Densities by Corresponding-States Correlation

Liquid-phase densities ρ were calculated with the extended corresponding-states equation of Riedel (54RIE), as formulated by Hales and Townsend (72HAL/TOW):

$$(\rho/\rho_c) = 1.0 + 0.85\{1.0 - (T/T_c)\} + (1.692 + 0.986\omega)\{1.0 - (T/T_c)\}^{1/3}, \quad (2)$$

with T_c , p_c , and ω from Table 1. The critical density ρ_c was adjusted to optimize agreement between the calculated and measured densities. The percentage deviations are listed in Table 3.

A comparison between the critical densities estimated here and those measured by Teja and co-workers (91GUD/ROS, 83WOL/KAY) and Peisheng *et al.* (91PEI/YOU) is shown in Fig. 1. Measured ρ_c values for the alkanes (90ANS/GUD) are shown, also. The trend with carbon number of the critical densities estimated here is in accord with that observed for the alkanes. The estimated values are slightly outside the uncertainty range claimed for the experimental values. The estimated ρ_c values were used for all density calculations to provide the best densities for the pressure range in which they were required (typically near or below 1 bar).

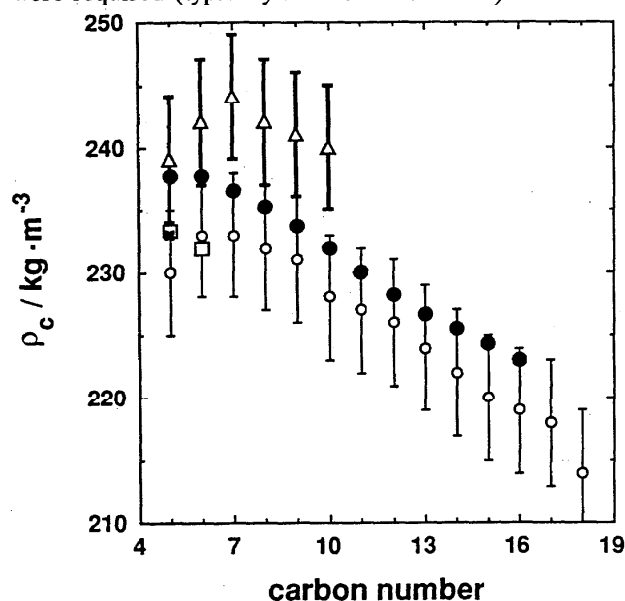


FIG. 1. Critical density ρ_c against carbon number. ●, values for normal alk-1-enes estimated in this review; Δ, values for normal alk-1-enes determined by Teja and co-workers (91GUD/ROS); □, pent-1-ene and hex-1-ene determined by Peisheng *et al.* (91PEI/YOU); x, pent-1-ene determined by Wolfe, Kay, and Teja (83WOL/KAY); ○, normal alkanes (90ANS/GUD).

2.3.c. Comparison of Measured and Calculated Densities

As noted earlier, few density studies for alkenes span an extended temperature range. Of the several exceptions to this generalization, the work of Kireev (74KIR) for the terminal alkenes from pent-1-ene through dec-1-ene, and the recent studies by Dymond *et al.* (88DYM/MAL) on oct-1-ene, Wolfe *et al.* (83WOL/KAY) on pent-1-ene, and Peisheng *et al.* (91PEI/YOU) on pent-1-ene, 3-methylbut-1-ene, and hex-1-ene are most notable.

Dymond *et al.* studied the (p, ρ, T) properties of oct-1-ene between 298.15 K and 373.15 K for pressures between 0.1 MPa and 315 MPa. For their low-pressure

results, the deviations from values derived from corresponding states [equation (2)] are all within the experimental error range.

Kireev (74KIR) determined densities along the saturation line for the C_5 through C_{10} 1-olefins by an ultrasound propagation method for temperatures between approximately 170 K and 470 K. The experimental density values and percentage deviations from values calculated with equation (2) are listed in Table 3. The percentage deviations are shown as function of reduced temperature in Fig. 2. For reduced temperatures between 0.4 and 0.75, the values measured by Kireev are in excellent accord (within 0.3 percent) with the values derived with equation (2). At higher and lower reduced temperatures, positive deviations are apparent; however, these never exceed 1 percent except for two values for pent-1-ene, which are within 20 K of the critical temperature.

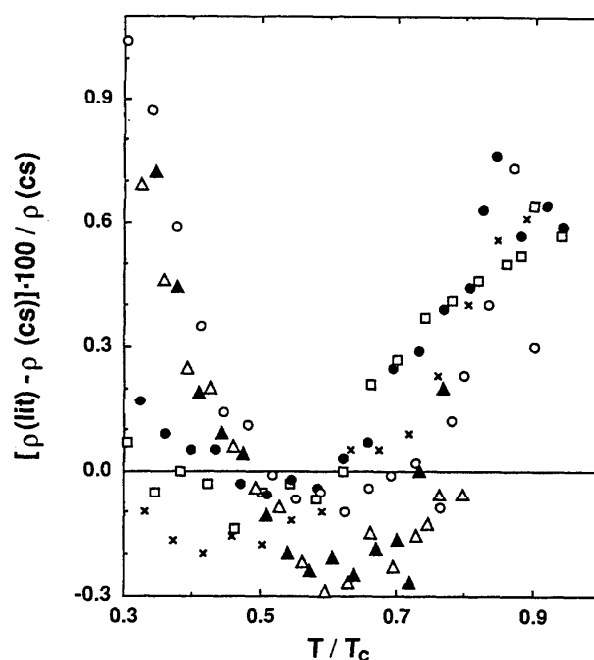


FIG. 2. Deviations of densities measured by Kireev (74KIR) from values calculated by corresponding states (cs) [equation (2)]. x, pent-1-ene; □, hex-1-ene; ●, hept-1-ene; ○, oct-1-ene; Δ, non-1-ene; ▲, dec-1-ene.

Wolfe *et al.* (83WOL/KAY) studied the (p, ρ, T) properties of pent-1-ene between 362.4 K and the critical temperature (near 465 K). The measured values are in good accord (within 0.5 percent) with those calculated with equation (2) for the entire temperature range.

Peisheng *et al.* (91PEI/YOU) determined saturation liquid densities for pent-1-ene, 3-methylbut-1-ene, and hex-1-ene at reduced temperatures between 0.80 and 0.99 with a precision of roughly 2 percent. The experimental results for pent-1-ene and 3-methylbut-1-ene are in good accord with those estimated with corresponding states (Eq. 2) as seen in Table 3. The experimental

and estimated density values for hex-1-ene diverge for reduced temperatures above 0.95. In Appendix 2 it is shown that the vapor pressures reported by Peisheng *et al.* for hex-1-ene, also, are not in good accord with values derived with the Cox-equation coefficients of Table 2, in contrast to the results for pent-1-ene and 3-methylbut-1-ene. The low purities of the materials used by Peisheng *et al.* {pent-1-ene, 99.2 percent; hex-1-ene 99.0 percent; and 3-methylbut-1-ene, 99.4 percent} could account for many of the observed discrepancies.

Curtice *et al.* (72CUR/FEL) measured densities between 122 K and 298 K for *cis*-pent-2-ene; however, the purity of the sample was low. The measured values are in only fair accord with the results calculated by corresponding states.

Seyer (31SEY) published densities for *cis*- and *trans*-pent-2-ene, and 2-methylbut-2-ene over broad temperature ranges. The pent-2-ene results are relative values only, in that they are based on an assumed density for 293.15 K. The trends in density with temperature are seen to be in good accord with the calculated values in Table 3 for the pent-2-enes. The results for 2-methylbut-2-ene deviate from the calculated values by from 0.7 percent near 300 K to 1.8 percent near 200 K. The values above 300 K are widely scattered. Adjustment of the critical parameters could improve the agreement for 2-methylbut-2-ene, but only at the expense of the accord shown later between experimental and derived enthalpies of vaporization. (See section 2.5.)

Jeffery and Vogel (48JEF/VOG) measured densities between approximately 290 K and 350 K for hex-1-ene, and between 290 K and 370 K for oct-1-ene, dec-1-ene, dodec-1-ene, tetradec-1-ene, and hexadec-1-ene. Except for the hex-1-ene results, which are 1 percent high, their values rarely differ from the corresponding-states results by more than 0.25 percent.

2.4. Second Virial Coefficients

2.4.a. Measured Second Virial Coefficients

There are only two reports (49SCO/WAD, 64MCG/WOR) of experimentally determined second virial coefficients in the literature for mono-olefins larger than C_4 . The measured values for the six compounds studied are listed in Table 4.

2.4.b. Estimation by Corresponding-States Correlation

Second virial coefficients were estimated with the corresponding-states equation of Pitzer and Curl (57PIT/CUR) and the critical-property values listed in Table 1. The agreement between the calculated and measured values is excellent.

2.5. Enthalpies of Vaporization

2.5.a. Measured Enthalpies of Vaporization

Enthalpies of vaporization have been determined directly for eight alkenes larger than C_4 . The measured val-

ues with the claimed uncertainties are listed in columns 1 and 2 of Table 5.

2.5.b. Estimation via the Cox and Clapeyron Equations

Enthalpies of vaporization $\Delta^f H_m$ were derived from the Cox equation fits to the selected measured vapor-pressures by means of the Clapeyron equation:

$$dp/dT = \Delta^f H_m / (T \Delta^f V_m) . \quad (3)$$

$\Delta^f V_m$ is the increase in molar volume from the liquid to the real vapor. The Cox-equation fits (Table 2) were employed to derive dp/dT . Estimates of liquid-phase volumes were made with equation (2). Vapor-phase volumes were calculated with the virial equation of state truncated at the third virial coefficient. Second virial coefficients were estimated with the corresponding-states equation of Pitzer and Curl (57PIT/CUR) and third virial coefficients were estimated with the corresponding-states method of Orbey and Vera (83ORB/VER). Third virial coefficients are required for accurate calculation of the gas volume for pressures greater than 0.1MPa. Uncertainties in the virial coefficients were assumed to be 10 percent. For $p > 0.1$ MPa the uncertainties in the virial coefficients are the dominant contributions to the uncertainties in the derived enthalpies of vaporization.

The enthalpies of vaporization derived from the Cox and Clapeyron equations and their estimated uncertainties are listed in column 3 of Table 5. The differences between the directly-measured and derived values are listed in column 4. The differences are all within the estimated uncertainties except for the measurements of Chickos *et al.* (81CHI/HYM), which do not include uncertainty estimates. The uncertainties of "lower than 0.2 percent" claimed by Svoboda *et al.* (82SVO/CHA) for their measurements on oct-1-ene were later shown by Majer and Svoboda (85MAJ/SVO) to be slightly optimistic. An uncertainty of 0.3 percent was used in Table 5.

2.5.c. Enthalpies of Vaporization at 298.15 K

The enthalpies of vaporization used for the calculation of enthalpies of formation for the gas phase state from enthalpies of combustion for the liquid phase are shown in Table 6. The source of each value is shown in column 3 of the table.

2.6. Enthalpies of Formation

2.6.a. Enthalpies of Combustion for the Liquid Phase

Measured enthalpies of combustion for the liquid phase of the alkenes at 298.15 K are listed in Table 7. The enthalpies of combustion of the hexenes (56BAR) were later published as relative values only (60BAR/ROS). The values listed by Pedley *et al.* (86PED/NAY) for *cis*- and *trans*-2-octene are estimates only (77PED/RYL) and are not experimentally-determined enthalpies of combustion as assumed by other authors (92ROG/DEJ, 88DOM/

HEA). All uncertainties listed in Table 7 are the "uncertainty interval" as defined in 56ROS. The value listed first for each compound was selected as the most reliable, and was used for all further calculations.

The enthalpy of formation for *cis*-hex-2-ene was adjusted approximately $4 \text{ kJ}\cdot\text{mol}^{-1}$ positive relative to the value derived from the enthalpy of combustion results (56BAR). Results of experimental equilibria (see section 3.7) and enthalpy-of-hydrogenation and hydration studies (see section 4.3) indicated that the enthalpy-of-combustion results were in error. The adjusted value was used for all further calculations.

2.6.b. Enthalpies of Formation for the Liquid Phase at 298.15 K

For conversion of the enthalpies of combustion to enthalpies of formation, the enthalpies of formation of $\text{CO}_2(\text{g})$ and $\text{H}_2\text{O}(\text{l})$ were taken to be $(393.51 \pm 0.13) \text{ kJ}\cdot\text{mol}^{-1}$, $-(285.830 \pm 0.042) \text{ kJ}\cdot\text{mol}^{-1}$, respectively, as assigned by CODATA (89COX/WAG). The derived enthalpies of formation for the liquid phase at 298.15 K are listed in column 4 of Table 7.

2.6.c. Enthalpies of Formation for the Gas at 298.15 K

The derived enthalpies of formation for the liquid phase at 298.15 K were combined with the enthalpies of vaporization listed in Table 6 to calculate the enthalpies of formation for the gas listed in the final column of Table 7. The enthalpies of formation for the gas are listed only for the enthalpy of combustion selected as most reliable.

2.7. Condensed-Phase Heat Capacities and Derived Functions

2.7.a. Measured Condensed-Phase Heat Capacities

For alkenes larger than C_4 , all condensed-phase heat-capacity studies, which extend to near 0 K (typically near 12 K), were obtained by the Thermodynamics Group in Bartlesville, OK. Earlier low-temperature heat-capacity studies by Parks and co-workers on hept-1-ene, 2,3-dimethylbut-2-ene (36PAR/TOD), and 3,3-dimethylbut-1-ene (38KEN/SHO) did not extend below 80 K, and are not suitable for accurate entropy determinations.

Pent-1-ene was studied initially by Todd *et al.* (47TOD/OLI). Later results obtained with a higher purity sample were published by Messerly *et al.* (90MES/TOD). These later results were used here. Differences between the results for the two samples are discussed in 90MES/TOD. Experimental results used in the present compilation for the remaining five pentenes are those of Todd *et al.* (47TOD/OLI).

Heat-capacity measurements between approximately 12 K and 320 K were completed for hept-1-ene, oct-1-

ene, dec-1-ene, undec-1-ene, dodec-1-ene, and hexadec-1-ene (57MCC/FIN). Results for *non*-1-ene and a higher purity sample of hexadec-1-ene were obtained by the same research group and published much later (90MES/TOD). The results for the two samples of hexadec-1-ene are compared in 90MES/TOD. The later results were used in all calculations here.

Cis-hex-2-ene (90MES/TOD) and 2,3-dimethylbut-2-ene (55SCO/FIN) are the only branched alkenes larger than C_5 that have been studied with adiabatic calorimetry to temperatures sufficiently low to calculate entropies relative to 0 K.

2.7.b. Condensed-Phase Heat Capacities, Enthalpies, and Entropies

All of the heat capacities obtained with adiabatic calorimetry for the alkenes (except those in 90MES/TOD) were published in terms of the 1948 temperature scale. The results published in 1990 were in terms of IPTS-68. When practical, all values were converted to ITS-90.

Conversion to ITS-90 involved determination of the initial and final temperature for each measured "heat-capacity" value, conversion of these values to ITS-90, and recalculation of the heat capacity with the new temperature increment. Polynomials were fit to the revised experimental heat capacities to provide values at even temperatures and to provide a means for integration. Differences between the heat capacities on the 1948 scale and ITS-90 were on the order of 0.1 percent. The effects on the derived entropies and enthalpies relative to 0 K for the liquid were approximately an order of magnitude smaller.

It is essential to realize that the reported "heat capacities" by adiabatic calorimetry are not measured directly. The reported values are average heat capacities over a defined temperature interval. Only if the temperature interval is known, can the temperature-scale conversion be accomplished.

Several of the alkenes (2,3-dimethylbut-2-ene; dec-1-ene; undec-1-ene; and dodec-1-ene) exhibit high-temperature crystalline phases with short temperature ranges. The uncertainties involved in the original data were too large to justify conversion of these results to ITS-90. Results for the low-temperature phase *cr*(II) and the liquid phase were converted to ITS-90. Only the results for the liquid phase of hexadec-1-ene were converted to ITS-90; the crystal-phase results are in terms of IPTS-68, as they were published in 1990 (90MES/TOD). Uncertainties associated with the multiple phase changes for this compound make conversion of the crystal-phase results to ITS-90 superfluous.

Condensed-phase heat capacities, and enthalpies and entropies relative to that of the crystals at 0 K are listed in Table 8. Liquid-phase heat capacities were extrapolated 50 K graphically for most materials. The values obtained by extrapolation are so indicated.

2.8. Thermodynamic Properties in the Ideal-Gas State

2.8.a. Derived Ideal-Gas Enthalpies and Entropies

Enthalpies and entropies at selected temperatures for the ideal gas were calculated using values in Tables 8 and the enthalpies of vaporization listed in Table 9, and are listed in columns 2 and 4 of Table 10. The enthalpies-of-vaporization values listed in Table 9 were calculated with the Cox and Clapeyron equations, as described in section 2.5.b. Entropies and enthalpies of compression to $p = 101.325 \text{ kPa}$ were calculated based on the virial equation truncated after the third virial coefficient:

$$pV_m = RT + Bp + Cp^2. \quad (4)$$

Formulations used to calculate the entropy and enthalpy of compression are (61LEW/RAN):

$$\Delta_{\text{comp}}S_m = R \ln(p/p^\circ) + (dB/dT)p + (dC/dT)p^2, \quad (5)$$

$$\Delta_{\text{comp}}H_m = \{B - T(dB/dT)\}p + \{C - T(dC/dT)\}(p^2/2). \quad (6)$$

Equations (5) and (6) are derived from Eqs. (16.21) and (16.27), respectively, of Ref. 61LEW/RAN. Temperature derivatives were estimated by numerical differentiation of virial coefficients estimated by the methods of Pitzer and Curl (57PIT/CUR) and Orbey and Vera (83ORB/VER).

The first term in Eq. (5) is the entropy of compression, if the gas is ideal. The uncertainty in this term is not significant. The sum of the second and third terms of Eq. (5) is the "gas-imperfection correction" to the entropy of compression. Eq. (6) gives the "gas-imperfection correction" to the enthalpy of compression directly, as the enthalpy of compression for an ideal-gas is zero. The gas-imperfection corrections are listed in columns 3 and 5, and are included in columns 2 and 4 of Table 10. Uncertainties in these values are difficult to assess because temperature derivatives of estimated values are involved. An uncertainty of 10 percent of the calculated correction was assumed.

2.8.b. Derived Ideal-Gas Formation Properties

The derived ideal-gas enthalpies and entropies were combined with the ideal-gas enthalpies of formation given in Table 7 to calculate the enthalpies, entropies, and Gibbs energies of formation listed in columns 6, 7, and 8, respectively, of Table 10. Enthalpies and entropies for equilibrium hydrogen were derived from JANAF tables (85CHA/DAV). Values for graphite were determined with the polynomial (90CHI/ARC) used to calculate the values from 298.15 K to 6000 K listed in the JANAF tables. All uncertainties in Table 10 represent one standard deviation and do not include uncertainties in the properties of the elements. Uncertainties in the properties of the elements were not included because they cancel in calculations of chemical equilibria. Their

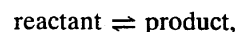
inclusion would lead to overestimation of the error limits in such calculations.

2.8.c. Ideal-Gas Entropies via Spectroscopy and Statistical Mechanics

Entropies for the ideal-gas states of 2-methylbut-1-ene (49SCO/WAD) and 2,3-dimethylbut-2-ene (55SCO/FIN) were calculated by Scott and co-workers from assigned spectra and statistical mechanics. Barrier heights for hindered rotors were adjusted to yield agreement with the calorimetric results; consequently, these are not independent values. The studies by Durig *et al.* (80DUR/GER, 81DUR/GER) exemplify the difficulties involved in the statistical calculation of thermodynamic properties for these materials.

3. Thermodynamic Equilibria

The calculation of thermodynamic equilibria in organic systems has been outlined in previous publications from this research group (90STE/CHI, 89STE/ARC, 87CHI/HOS). The methodology can be summarized as follows. For the general reaction:



the equilibrium constant, K , is approximately:

$$K = [p_{\text{product}} / p_{\text{reactant}}], \quad (7)$$

and the Gibbs energies of formation, $\Delta_f G_m^\circ$, for reactants and products are directly related to the equilibrium constant through the relations:

$$\begin{aligned} \sum \Delta_f G_m^\circ(\text{products}) - \sum \Delta_f G_m^\circ(\text{reactants}) \\ = \Delta_r G_m^\circ = -RT \ln K. \end{aligned} \quad (8)$$

[In a more rigorous treatment, the partial pressures are replaced by fugacities. For most experimental conditions (see Figs. 3 through 7, and 9), the difference is not significant.] If $\ln K$ is plotted versus $1/T$, near linear curves are obtained. This facilitates extrapolation of the experimental values obtained at relatively low temperature into the range of commercial processes. $\Delta_r G_m^\circ$ can be split into an enthalpy and entropy contribution. Then, equation (8) can be written:

$$\ln K = -\Delta_r H_m^\circ/RT + \Delta_r S_m^\circ/R. \quad (9)$$

Thus, the slope of a $\ln K$ versus $1/T$ plot is directly proportional to the enthalpy of reaction, $\Delta_r H_m^\circ$.

3.1 Pent-1-ene \rightleftharpoons *trans*-Pent-2-ene Equilibria

Figure 3 summarizes the results for the pent-1-ene \rightleftharpoons *trans*-pent-2-ene equilibrium obtained using the method described above. The calorimetrically determined values for both pentenes cover only the tempera-

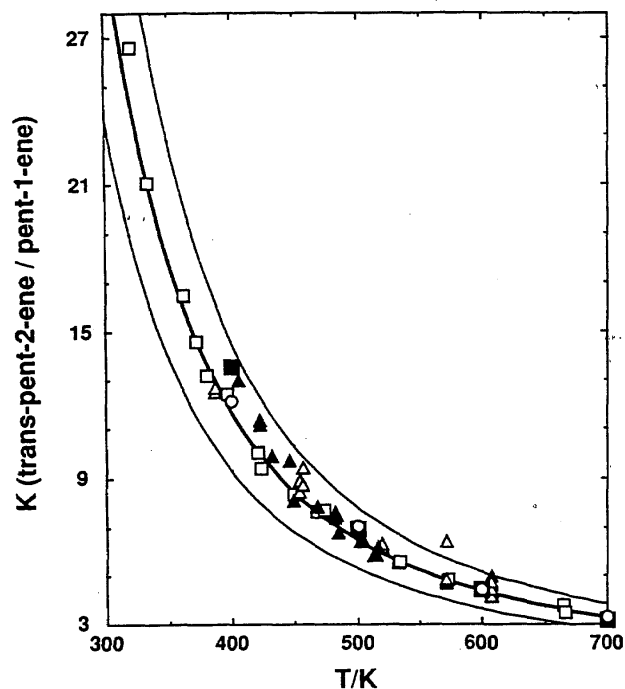


FIG. 3. Equilibrium constants versus temperature for the equilibrium pent-1-ene \rightleftharpoons *trans*-pent-2-ene. The plot compares values obtained in experimental studies on the equilibrium with values derived (see text) using the ideal-gas thermodynamic properties listed in Table 10. The center curve represents the calculated equilibria derived using the values from Table 10. The upper and lower curves represent the boundaries of one standard deviation in the calculated equilibrium constant. \square , 75COR/VEL; Δ , 66EGG/BEN; \blacktriangle , 68KAR/AND. Also included for comparison are values derived using the ideal-gas thermodynamic properties listed in 69STU/WES (\blacksquare) and 90TRC(O).

ture range 250 to 350 K. The center curves plotted in Figs. 3 through 7 represent the variation of the equilibrium constant with temperature derived from the values reported in Table 10. The equation of the curve in Fig. 3 is:

$$K = \exp[1191 (K/T) - 0.515]. \quad (10)$$

The upper and lower curves in Figs. 3 through 7 represent the bounds of the equilibrium constant calculated using the uncertainty limits (one standard deviation) assigned to the Gibbs energies in Table 10.

The comparisons shown in Fig. 3 involve a large extrapolation for the values derived with the Gibbs energies of formation, but the agreement with the equilibrium studies is still excellent with all but a single determination of the equilibrium constant lying within the uncertainty bounds.

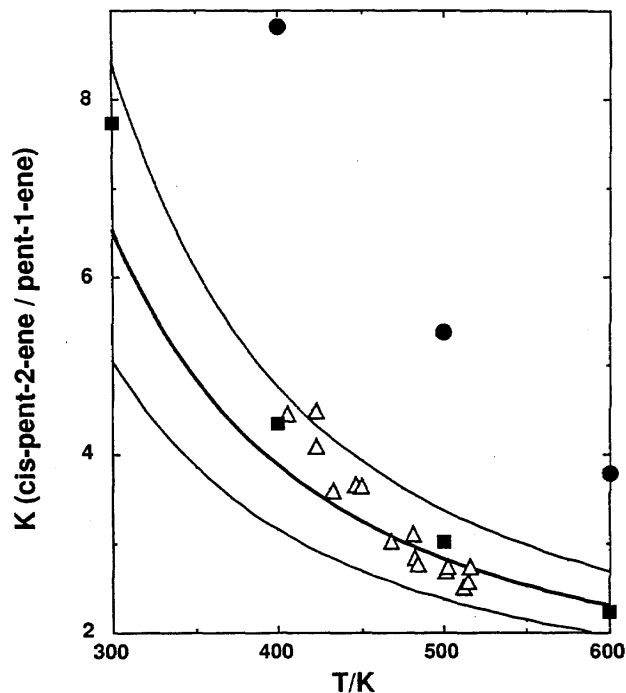


FIG. 4. Equilibrium constants versus temperature for the equilibrium pent-1-ene \rightleftharpoons *cis*-pent-2-ene. The plot compares values obtained in experimental studies on the equilibrium with values derived (see text) using the ideal-gas thermodynamic properties listed in Table 10. The center curve represents the calculated equilibria derived using the values from Table 10. The upper and lower curves represent the boundaries of one standard deviation in the calculated equilibrium constant. Δ , 68KAR/AND. Also included for comparison are values derived using the ideal-gas thermodynamic properties listed in 69STU/WES (\bullet) and 90TRC(\blacksquare).

3.2. Pent-1-ene \rightleftharpoons *cis*-Pent-2-ene Equilibria

Figure 4 summarizes the results for the *cis*-pent-2-ene \rightleftharpoons *trans*-pent-2-ene equilibrium. The calorimetrically determined values for both pentenes cover only the temperature range 250 to 350 K. The variation of the equilibrium constant with temperature derived from the values reported in Table 10, is expressed as:

$$K = \exp[627.0 (K/T) - 0.214]. \quad (11)$$

The comparisons again involve a long extrapolation for the values derived using the Gibbs energies of formation, but the agreement with the equilibrium studies (68KAR/AND) is still excellent. The relatively large deviation of the results based on 69STU/WES should be considered in light of the fact that the Gibbs-energy values listed in 69STU/WES are slight modifications of values estimated within API Project 44 (53ROS/PIT), which was compiled prior to the completion of many of the measurements used to calculate the Gibbs energies in Table 10.

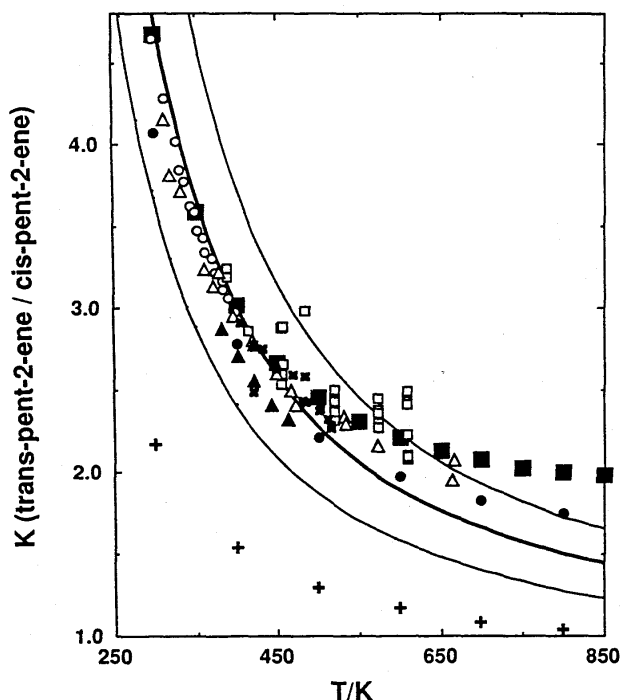


FIG. 5. Equilibrium constants versus temperature for the equilibrium $\text{cis-pent-2-ene} \rightleftharpoons \text{trans-pent-2-ene}$. The plot compares values obtained in experimental studies on the equilibrium with values derived (see text) using the ideal-gas thermodynamic properties listed in Table 10. The center curve represents the calculated equilibria derived using the values from Table 10. The upper and lower curves represent the boundaries of one standard deviation in the calculated equilibrium constant. ■, 83KAP/STE; Δ , 75COR/VEL; \circ , 72AKI/SPR; x, 68KAR/AND; \blacktriangle , 66ABE; \square , 66EGG/BEN; Also included for comparison are values derived using the ideal-gas thermodynamic properties from 69STU/WES (+) and 90TRC (\bullet).

3.3. *cis*-Pent-2-ene \rightleftharpoons *trans*-Pent-2-ene Equilibria

Figure 5 summarizes the results for the *cis*-pent-2-ene \rightleftharpoons *trans*-pent-2-ene equilibrium. The calorimetrically determined values for both pentenes cover only the temperature range 250 to 350 K. The variation of the equilibrium constant with temperature derived from the values reported in Table 10, is expressed as:

$$K = \exp[563.6 (K/T) - 0.301]. \quad (12)$$

The upper and lower curves in Fig. 5 represent the bounds of the equilibrium constant calculated using the uncertainty limits (one standard deviation) assigned to the Gibbs energies in Table 10.

The comparisons again involve a long extrapolation for the values derived using the Gibbs energies of formation, but the agreement with the equilibrium studies is still excellent, particularly for values below 500 K. Above 500 K, the experimental equilibrium constants are systematically

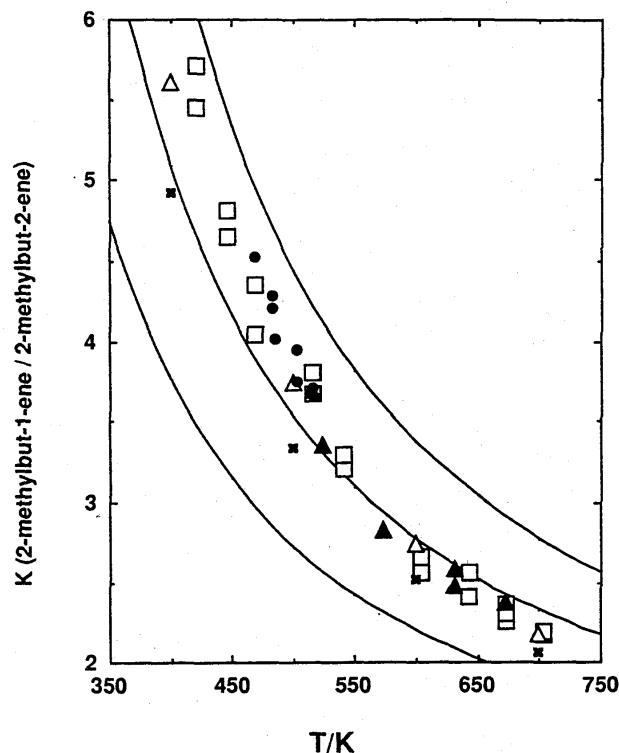


FIG. 6. Equilibrium constants versus temperature for the equilibrium $2\text{-methylbut-1-ene} \rightleftharpoons 2\text{-methylbut-2-ene}$. The plot compares values obtained in experimental studies on the equilibrium with values derived (see text) using the ideal-gas thermodynamic properties listed in Table 10. The center curve represents the calculated equilibria derived using the values from Table 10. The upper and lower curves represent the boundaries of one standard deviation in the calculated equilibrium constant. \square , 73RAD/KAB; \bullet , 68KAR/AND; \blacktriangle , 41EWE/HAR. Also included for comparison are values derived using the ideal-gas thermodynamic properties from 69STU/WES(Δ) and 90TRC(x).

high relative to the thermodynamic calculations. New high-temperature heat-capacity measurements would help resolve the discrepancy. The relatively large deviation of the results based on 69STU/WES should again be considered in light of the fact that the Gibbs-energy values listed in 69STU/WES are slight modifications of values estimated within API Project 44 (53ROS/PIT).

3.4. 2-Methylbut-1-ene \rightleftharpoons 2-Methylbut-2-ene Equilibria

Figure 6 summarizes the results for the 2-methylbut-1-ene \rightleftharpoons 2-methylbut-2-ene equilibrium. Again, the calorimetrically determined values for both pentenes cover only the temperature range 250 to 350 K. The variation with temperature of the equilibrium constant K , based on the Gibbs energies of Table 10, is expressed as:

$$K = \exp[729 (K/T) - 0.196]. \quad (13)$$

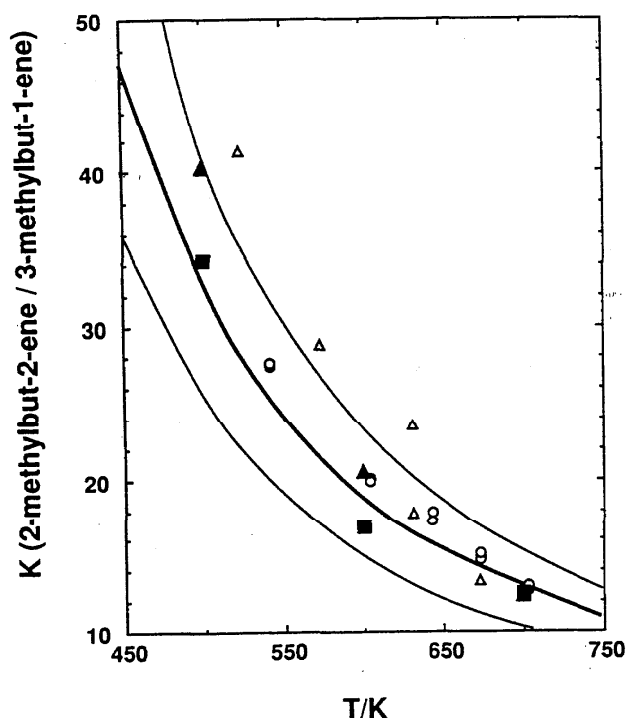


FIG. 7. Equilibrium constants versus temperature for the equilibrium 3-methylbut-1-ene \rightleftharpoons 2-methylbut-2-ene. The plot compares values obtained in experimental studies on the equilibrium with values derived (see text) using the ideal-gas thermodynamic properties listed in Table 10. The center curve represents the calculated equilibria derived using the values from Table 10. The upper and lower curves represent the boundaries of one standard deviation in the calculated equilibrium constant. \circ , 73RAD/KAB; Δ , 41EWE/HAR. Also included for comparison are values derived using the ideal-gas thermodynamic properties from 69STU/WES(\blacktriangle) and 90TRC(\blacksquare).

The comparisons involve long extrapolation for the values derived using the Gibbs energies of formation, but the agreement with the equilibrium studies remains excellent.

3.5. 3-Methylbut-1-ene \rightleftharpoons 2-Methylbut-2-ene Equilibria

Figure 7 summarizes the results for the 3-methylbut-1-ene \rightleftharpoons 2-methylbut-2-ene equilibrium. The center curve plotted in Fig. 7 represents the variation of the equilibrium constant with temperature derived from the values reported in Table 10, that, again, cover only the temperature range 250 to 350 K. The equation of the curve is:

$$K = \exp[1734 (K/T) + 0.243]. \quad (14)$$

The agreement between the calorimetrically-derived values and the equilibrium studies reported in 73RAD/

KAB is excellent. The agreement with the earlier study (41EWE/HAR) is less so, with several of the values lying outside the single standard-deviation "error" bounds.

3.6. Pentenes Equilibria Summary

Figure 8 summarizes the results of calculations of the mole percent composition for all the pentenes under thermodynamic equilibria over the temperature range 300 to 800 K. Equations (10) through (14) were used to obtain the respective mole percentages at equilibrium.

Zharkova and Moldavskii (48ZHA/MOL) determined equilibria for the pentenes at 473 K and 653 K, however, they did not fully separate the product mixture. Results are reported for three components; 3-methylbut-1-ene, [pent-1-ene + *cis*-pent-2-ene + *trans*-pent-2-ene], and [2-methylbut-2-ene + 2-methylbut-1-ene]. At 473 K, they report the following mole percentages: 3.3 (0.8), 19.0 (27.8), and 77.7 (71.3), respectively. Values in brackets are percentages calculated with equations (10) through (14). At 653 K, they report mole percentages: 7.1 (2.4), 28.2 (37.1), and 64.7 (60.5), respectively. Agreement between the experimental and calculated results is not as good as for later results such as 73RAD/KAB, 75COR/VEL, 68KAR/AND, etc.

3.7. Hex-1-ene \rightleftharpoons *cis*-Hex-2-ene Equilibria

Figure 9 summarizes the results for the hex-1-ene \rightleftharpoons *cis*-hex-2-ene equilibrium obtained using the method described above. The calorimetrically determined values for both hexenes cover only the temperature range 250 to 350 K. The center curve plotted in Fig. 9 represents the variation of the equilibrium constant with temperature derived from the values reported in Table 10. The equation of the curve is:

$$K = \exp[688 (K/T) + 0.068]. \quad (15)$$

The agreement of the calorimetrically-derived values with the equilibrium studies reported by Maurel *et al.* (69MAU/GUI) for temperatures from 473 K to 673 K is excellent, if the revised value for the enthalpy of combustion of *cis*-hex-2-ene is used in the thermodynamic calculations. The "+" symbols show the results of the thermodynamic calculations, if the enthalpy of combustion reported by Bartolo (56BAR) is employed.

Maurel *et al.* (69MAU/GUI) also investigated equilibria between the mono-methyl pentenes. There is insufficient experimental thermodynamic information to calculate Gibbs energies for these materials.

4. Comparisons with Hydrogenation and Isomerization Studies

4.1. Enthalpies of Hydrogenation

The modern era in the measurement of enthalpies of hydrogenation of unsaturated organic compounds started

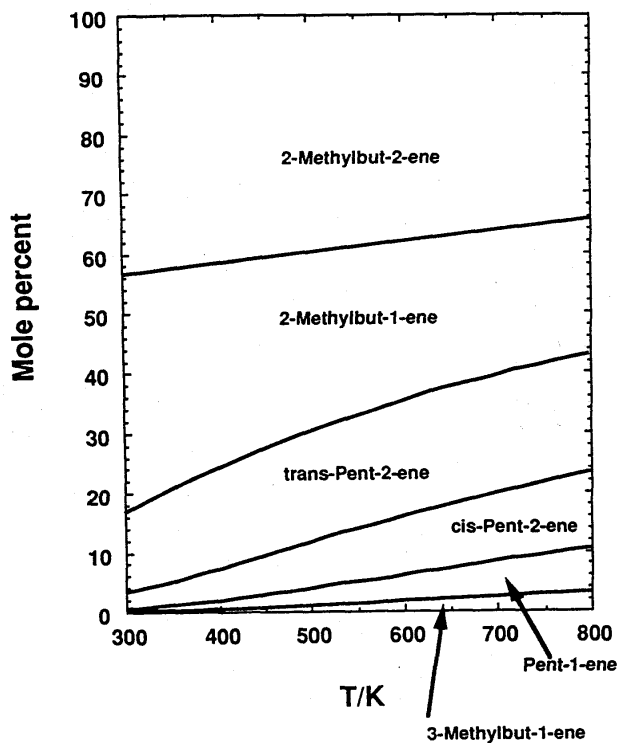


FIG. 8. Equilibrium mole per cent versus temperature for the six pentenes. The plot was derived using the ideal-gas thermodynamic properties listed in Table 10.

with the work of Kistiakowsky and his group at the Microcalorimetric Chemical Laboratory at Harvard University (35KIS/ROM). Prior to that pioneering work on ethylene, many – if not all – reports of enthalpy-of-hydrogenation measurements are of historical interest only. Kistiakowsky and his group made careful hydrogenation reaction-calorimetric measurements on many unsaturated compounds. The published studies relevant to this review are 36KIS/RUH and 37DOL/GRE. (It should be noted that Kistiakowsky and his group worked with compounds in the gas phase at 355 K and not at 298.15 K, as is often assumed.) In 36KIS/RUH and 37DOL/GRE results are reported for the enthalpies of hydrogenation of hept-1-ene, 4-methyl-*trans*-pent-2-ene, 2-methylbut-2-ene, 2,3-dimethylbut-2-ene, 3-methylbut-1-ene, 4,4-dimethylpent-1-ene, 3,3-dimethylbut-1-ene, 2,4,4-trimethylpent-1-ene, and 2,4,4-trimethylpent-2-ene.

It is not within the scope of this project to assess the thermodynamic properties of the alkanes (i.e., the hydrogenation products), so calculations of the enthalpies of formation of the alkenes were not made based on the enthalpy-of-hydrogenation results. Instead, here and in subsequent sections, comparisons are made between derived enthalpies of isomerization and values obtained by combustion calorimetry (combined with enthalpies of vapor

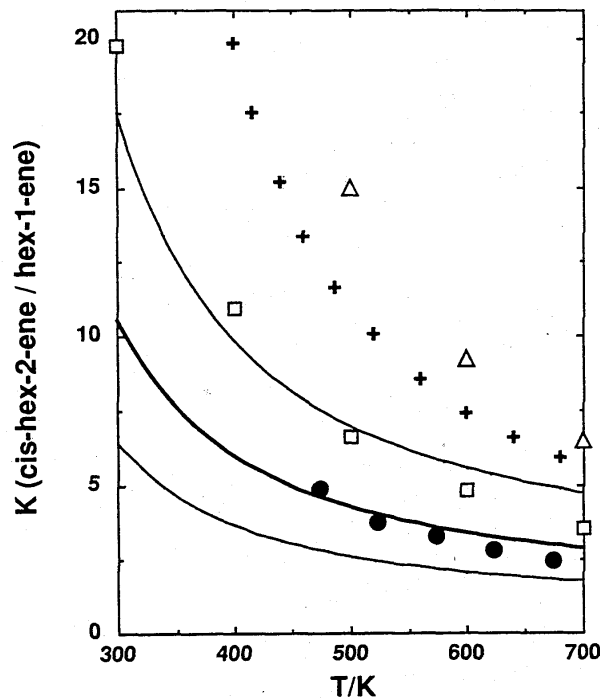


FIG. 9. Equilibrium constants versus temperature for the equilibrium $\text{hex-1-ene} \rightleftharpoons \text{cis-hex-2-ene}$. The plot compares values obtained in experimental studies on the equilibrium with values derived (see text) using the ideal-gas thermodynamic properties listed in Table 10. The center curve represents the calculated equilibria derived using the values from Table 10. The upper and lower curves represent the boundaries of one standard deviation in the calculated equilibrium constant. ●, 69MAU/GUI experimental equilibria results. Also included for comparison are values derived using the ideal-gas thermodynamic properties listed in 69STU/WES(Δ) and 90TRC(\square). The +’s show the results of the thermodynamic-equilibria calculations, if the enthalpy of combustion of Bartolo (56BAR) was used in the calculation rather than the adjusted value listed in Table 7. (See section 3.7 and 4.3 of the text.)

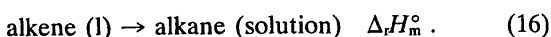
ization, if values for the gas phase are required). This is possible when the product of the reaction – in this case hydrogenation – is the same for two or more compounds.

For example, of the olefins studied by Kistiakowsky and his group, a comparison can be made for two pairs of compounds: 2-methylbut-2-ene/3-methylbut-1-ene, and 2,4,4-trimethylpent-1-ene/2,4,4-trimethylpent-2-ene. The first pair produce 2-methylbutane on hydrogenation and the second pair form 2,2,4-trimethylpentane. For the 2-methylbut-2-ene/3-methylbut-1-ene isomerization, the enthalpy based on the hydrogenation studies (36KIS/RUH) is $-14.2 \pm 0.36 \text{ kJ}\cdot\text{mol}^{-1}$ at 355 K. From Table 10 a value of $-13.42 \pm 1.84 \text{ kJ}\cdot\text{mol}^{-1}$ at 350 K is derived in excellent agreement with the hydrogenation work. (The 5 K difference in experimental temperature is not significant.) For the 2,4,4-trimethylpent-1-ene/2,4,4-trimethylpent-2-ene isomerization, the enthalpy based on the hydrogenation studies (37DOL/GRE) is $-4.84 \pm 0.36 \text{ kJ}\cdot\text{mol}^{-1}$ at 355 K. From Table 10 a value of

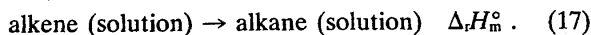
$-4.88 \pm 2.18 \text{ kJ}\cdot\text{mol}^{-1}$ at 298.15 K is derived, again in excellent accord. (The heat capacities necessary to adjust this value to 355 K are not available.)

Most reported enthalpies of hydrogenation subsequent to the work by Kistiakowsky's group have been made in organic solvent media at 298.15 K. Williams (42WIL) made careful studies in glacial acetic acid at 302 K on several unsaturated compounds including hept-1-ene. Turner *et al.* (58TUR/NET, 73TUR/JAR) reported enthalpies of hydrogenation in glacial acetic acid for several "crowded" olefins including *cis*- and *trans*-2,5,5-trimethylhex-3-ene, and *cis*- and *trans*-2,2,5,5-tetramethylhex-3-ene.

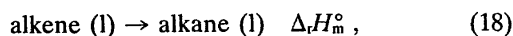
In most calorimetric measurements of enthalpies of hydrogenation, either an ampoule of the olefin is broken into a solvent containing a suspension of catalyst, or a solution of the olefin in the solvent is introduced into the catalyst/solvent mixture. In the first case the measured reaction enthalpy is represented by:



In the second case the measured reaction enthalpy is represented by:



In either case, to derive the enthalpy of reaction for the pure component liquid phase:

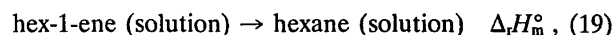


the enthalpy of solution of the alkane product in the solvent media is required. When the olefin is introduced in solution, the corresponding enthalpy of solution for the olefin is required, also. That enthalpy of solution is included in the measured energy of reaction, when the pure alkene is introduced into the solvent.

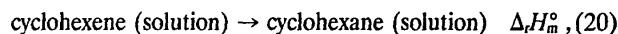
A widely accepted view has been that neglect of the enthalpies of solution for the reactants and products in the solvent media introduces little or no error in the derivation of enthalpies of formation. Skinner (59SKI/SNE) suggested that the enthalpy-of-solution correction to the enthalpy of hydrogenation of hex-1-ene in glacial acetic acid does not exceed the uncertainty in the enthalpy-of-reaction measurement, $\pm 0.8 \text{ kJ}\cdot\text{mol}^{-1}$. Fuchs and Peacock (79FUC/PEA1) made a detailed study of the enthalpies of solution of unsaturated compounds and their products of hydrogenation in the various solvents used by earlier researchers (glacial acetic acid, *n*-hexane, and cyclohexane). Results showed enthalpies of solution of various alkanes in glacial acetic acid as high as $10.8 \text{ kJ}\cdot\text{mol}^{-1}$ pointing to the possibility of large errors, if the enthalpy-of-solution corrections were ignored. The analogous error, if alkane solvents were used, was much smaller, but could still be as much as $0.5 \text{ kJ}\cdot\text{mol}^{-1}$.

Rogers *et al.* have made measurements of the enthalpies of hydrogenation of numerous olefins (70BRE/ROG, 71ROG/MCL, 74ROG/SKA, 75ROG/PAP, 79ROG, 83ROG/CRO, 84ROG/MUN, 87ROG/CRO, 88ROG/DEJ, 89ROG/DEJ, and 92ROG/DEJ). (Note:

79ROG is a correction to the results on 1-olefins published in 74ROG/SKA.) In the early work (70BRE/ROG) glacial acetic acid was used as the solvent, the pure olefin was introduced to the solvent media, and the enthalpy of reaction was determined relative to electrical calibration of the apparatus. In subsequent papers (71ROG/MCL, 74ROG/SKA, 75ROG/PAP, 79ROG, and 83ROG/CRO) the solvent was changed to *n*-hexane, and the results were derived relative to a selected value for the enthalpy of hydrogenation of hex-1-ene (i.e., the energy of reaction of hex-1-ene in the solvent media was used to calibrate the apparatus). Therefore, to obtain absolute values for the enthalpies of formation of the olefins studied, a value for the reaction:



was required. The problems involved in the determination of a "standard" value for this enthalpy of reaction are outlined in 79ROG. In subsequent papers (84ROG/MUN, 87ROG/CRO, 88ROG/DEJ, 89ROG/DEJ and 92ROG/DEJ) the standard reaction used to derive the enthalpy-of-hydrogenation results was changed to:



with Rogers *et al.* selecting a value of $-119.0 \text{ kJ}\cdot\text{mol}^{-1}$ for the reaction. Throughout the later papers, Rogers *et al.* make reference to enthalpies of solution being negligible, but do not give supporting evidence or refer to the careful measurements of Fuchs and Peacock (79FUC/PEA1).

As stated above, in this review absolute values of the enthalpies of formation of the olefins studied by hydrogenation reaction calorimetry are not derived. Instead, only comparisons of derived enthalpies of isomerization (when the product of the reaction for two or more compounds is the same alkane) with values obtained by combustion calorimetry are made. Table 11 lists the results of these comparisons. Discussion of the results is given below in Sec. 4.3.

4.2. Enthalpies of Hydration

In a series of papers published over the last decade, Wiberg and co-workers have measured enthalpies of hydration of a number of olefinic compounds. References 81WIB/WAS, 84WIB/WAS, and 91WIB/HAO are relevant to the topic of this review. Enthalpies of trifluoroacetylation of the olefins were measured in a solvent consisting of trifluoroacetic acid and 0.25M trifluoroacetic anhydride in the presence of a strong acid catalyst. Close attention was paid to the reactions occurring in the calorimetric solution and corrections made were appropriate to obtain a final state in which the ratio of trifluoroacetates was the same across the range of isomeric olefins under study. Table 11 lists values for the enthalpies of isomerization for cases where common reaction products are formed.

4.3. Comparison of Enthalpies of Isomerization

The enthalpies of isomerization given in Table 11 are not corrected for the enthalpies of solution of the olefins in the reaction solvent. However, some pertinent conclusions can still be made from the results. (Since the enthalpies are relevant to the same reaction product(s), the enthalpy of solution of the product(s) cancels in the enthalpy-of-isomerization calculations.)

First, contrary to a belief stated in most papers on reaction calorimetry, combustion calorimetric measurements can give enthalpies of isomerization as accurate (if not as precise) as those obtained in the most careful reaction calorimetry. Proof of this assertion can be seen, if the results listed in Table 11 for the C₅ and C₇ olefins are considered. In both cases the combustion calorimetric work was performed by Good and co-workers at Bartlesville (79GOO/SMI and 76GOO). Also, contrary to the statement made by Rogers in several of his recent papers (cf; 87ROG/CRO, 92ROG/DEJ), the size of the compounds studied by combustion calorimetry (at least up to C₈) does not affect the accuracy. For combustion calorimetric measurements the precision decreases as the molecular weight increases.

The combustion calorimetric measurements for the C₆ compounds listed in Table 11 were made by Bartolo and Rossini (56BAR, 60BAR/ROS). It appears that within those measurements at least some of the enthalpies of combustion may be in error by up to 4 kJ·mol⁻¹. This is most clearly true for *cis*-hex-2-ene, as corroborated by the experimental equilibria results for the hex-1-ene/*cis*-hex-2-ene equilibria (Sec. 3.7.). Other compounds with such errors may include *trans*-hex-3-ene and 2-methylpent-2-ene. However, there is insufficient experimental information available at this time to substantiate this assertion. In Sec. 5.2 it will be shown that the enthalpy of formation for 2-methylpent-2-ene appears to be 4 kJ·mol⁻¹ too negative based on a group-contribution analysis.

A value of -1.2 ± 0.3 kJ·mol⁻¹ is derived for the reaction *cis*-3-methylpent-2-ene → *trans*-3-methylpent-2-ene (not included in Table 11) from the results given in (91WIB/HAO). The corresponding value derived with the results of Rogers *et al.* (87ROG/CRO) is -0.5 ± 1.0 kJ·mol⁻¹. Combustion-calorimetry results give -0.4 ± 1.9 kJ·mol⁻¹. Hence, there may be in an error of 2 kJ·mol⁻¹ in the enthalpy of combustion of 3-methylpent-1-ene, but not in either of the 4-methylpent-2-ene isomers.

5. Comparison of Results with Group-Additivity Estimates at 298.15 K

5.1. Background (A Brief Historical Perspective)

Group-additivity methods for the estimation of thermodynamic properties have existed in various forms for more than seventy years; the first being introduced by Fa-

jans in 1920 (39PAU). Early methods employed single transferable bond energies and were not very successful. The additivity of structural group contributions was first shown by Parks and Huffman (32PAR/HUF), and was later formalized by Benson and Buss (58BEN/BUS). The Benson-type method as described in "Thermochemical Kinetics" (76BEN) is the most widely known and used estimation scheme today, and most other schemes can be reduced to it. The most recent published update of the Benson-type group-additivity parameters are those listed by Reid, Prausnitz, and Poling (87REI/PRA) in their Table 6-4. The updated parameters were used in the comparisons described in the following section.

5.2. Comparison with Updated Benson-type Group-Contribution Estimates

Tables 12 and 13 compare the experimentally-determined ideal-gas enthalpies of formation and entropies at 298.15 K with values derived by summation of group-additivity terms. No attempt was made to change individual group-additivity terms because they are closely interconnected with terms for the alkanes. However, the correction terms for *cis* interactions, when calculating enthalpies of formation, were reassessed and the following revised values used:

<i>cis</i> -alkyl group interaction	revised:	6.5 kJ·mol ⁻¹
	original:	4.2 kJ·mol ⁻¹

and:

<i>cis</i> -alkyl group interaction, if one group is a	
<i>tert</i> -butyl:	19.0 kJ·mol ⁻¹
original:	none given.

The only change made to the groups listed in 87REI/PRA for the calculation of ideal-gas entropies was:

<i>cis</i> -alkyl group interaction	revised:	0.46 R.
	original:	0.0

(Note: For this correction 76BEN states, "+1.2 cal·K⁻¹·mol⁻¹ for but-2-ene, 0 for all other 2-enes, and -0.6 for 3-enes." In 87REI/PRA this was transcribed incorrectly as, "value is 1.2 for but-2-ene, but 0 for other *dienes*, and 0.6 for *trienes*." The italics were added here. Also, the values listed in 87REI/PRA are meant to be in units of J·K⁻¹·mol⁻¹, while those listed in 76BEN are in cal·K⁻¹·mol⁻¹.)

As seen in Table 12, the agreement between the measured ideal-gas enthalpies of formation and those estimated by summation of the groups is generally excellent. Differences are usually within the uncertainty intervals on the measured values. Compounds where the difference is beyond the uncertainty interval include 2-methylpent-2-ene, *trans*-3-methylhex-3-ene, 3-methyl-2-ethylbut-1-ene, 2,3,3-trimethylbut-1-ene, and 2-methyl-3-ethylhex-1-ene. For 2-methylpent-2-ene, the differences are in accord with the assessment made above in the Enthalpies of Isomerization Section (Sec. 4.3).

As can be seen in Table 13, the agreement between the experimentally determined ideal-gas entropies at 298.15 K and those estimated by summation of the groups is fair for compounds smaller than C₁₂. For comparison, the excellent results for the analogous alkanes are shown.

The large differences for dodec-1-ene (-0.62R) and hexadec-1-ene (-0.64R) result from disorder in the crystalline form of these compounds at 0 K. If complete end-to-end disorder is present, the entropy of the disordered form is expected to be 0.69 R (i.e., R·ln2) lower than the ordered form. The effect can be observed most clearly, if the differences between the entropies at 298.15 K for the liquid normal alkanes and alk-1-enes are plotted against carbon number, as first noted by McCullough *et al.* (57MCC/FIN). These differences are plotted in Fig. 10 along with the analogous differences for the ideal-gases. The gas-phase results show a greater scatter because derivations of the enthalpies of vaporization for the alk-1-enes larger than C₇ involve significant vapor-pressure extrapolations. Reliable vapor pressures below 6.5 kPa are required for these larger alkenes.

2,3-Dimethylbut-2-ene contains two *cis* interactions and may need a different "cis correction." Study of at least another alkene with this type of substitution pattern is needed.

5.3. A Comment on the Correlation of Correlated Data

Recently, new group-contribution parameters were proposed for thermodynamic properties of the solid, liquid, and ideal-gas states of hydrocarbons at 298.15 K (88DOM/HEA). Comparison with the condensed-phase estimates is beyond the scope of this project. Values listed in 88DOM/HEA as "experimental" ideal-gas entropies for the alkenes are those given by Stull, Westrum, and Sinke in their monograph (69STU/WES). In 69STU/WES the authors stated clearly that the values of the API Project 44 (53ROS/PIT) were "selected" and listed. The values listed in 53ROS/PIT are updated estimates stemming from an earlier publication (46KIL/PRO), which pre-dates all of the measured vapor pressures and measured heat capacities used in this review. Therefore, the "experimental" values listed in 88DOM/HEA for ideal-gas entropies of alkenes are themselves derived from an additivity scheme. The authors have derived a correlation of a correlation, which is based on outdated information. This demonstrates the risk of using secondary sources in the development of correlations.

6. Overview of Database "Gaps" and the Need for New Experiments

6.1. Critical Properties Data Needs

Critical-property determinations for alkenes are extremely rare. The recent measurements by Peisheng *et al.* (91PEI/YOU) on 3-methylbut-1-ene and those of Kiyama

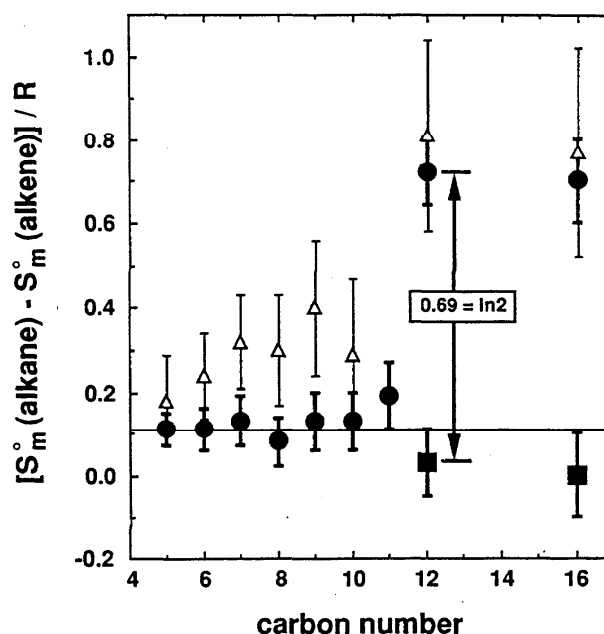


FIG. 10. Entropy differences at 298.15 K between the normal alkenes and the analogous alk-1-enes. ●; liquid-phase differences; ■, C₁₂ and C₁₆ liquid-phase differences with R·ln2 added to the dodec-1-ene and hexadec-1-ene entropy (see text); △, ideal-gas differences.

et al. (51KIY/SUZ) for 2-methylbut-2-ene are the only experimental critical properties reported for branched alkenes. [This includes the butenes, which were outside the scope of this review. In the review by Kudchadker *et al.* (68KUD/ALA) critical properties for *cis*- and *trans*-but-2-ene only are cited.] Except for the values determined by Lenior *et al.* (71LEN/REB) for *cis*-pent-2-ene and the two branched pentenes mentioned above, only terminal alkenes have been studied for carbon numbers larger than C₄.

The critical temperature measured for 2-methylbut-2-ene (51KIY/SUZ) is approximately 14 K lower than the value predicted by the estimation method of Joback (84JOB). The experimental *T_c* and *p_c* values were adopted in this research because their use yielded excellent accord between enthalpies of vaporization from vapor-flow calorimetry (49SCO/WAD) and those derived from the Cox-equation fits. (See Table 5.)

The scarcity of experimental critical properties for the alkenes puts group-contribution estimates, such as those used for most of the compounds in this review, on a weak foundation. Also, measured values for properties that can be estimated accurately by corresponding-states methods (i.e., densities and second virial coefficients) are available for too narrow a temperature range, too few compounds, or both, to allow some measure of the quality of the estimated *T_c* and *p_c* values.

6.2. Vapor Pressure Data Needs

Although vapor pressure results have been published for many straight-chain and branched alkenes, the values rarely extend above 1 bar or below 0.2 bar. Those few studies that do extend outside of this range are in poor to fair accord with the API-project results selected in this review (see Appendix 1).

Figure 11 shows the vapor-pressure and liquid-phase heat-capacity data ranges in terms of reduced temperature for compounds for which sufficient information is available to calculate ideal-gas properties for a range of temperatures. (The x's indicate 298.15 K.) For compounds larger than C₆ (except for non-1-ene) the ranges do not overlap and extrapolations must be used in the calculations. Additional vapor-pressure results for $p < 0.2$ bar would be valuable.

6.3. Enthalpy of Combustion Data Needs

In Sec. 5.2 it was demonstrated that the thermochemical data for the alkenes is generally in good accord. However, measurements are still needed for "strained" olefins in which the double bond is substituted with relatively bulky substituents such as tertiary butyl groups. Also, the energies of combustion for non-1-ene and undec-1-ene should be measured to complete the experimental determination of the ideal-gas properties of these compounds.

6.4. Condensed-Phase Heat Capacity Data Needs

Only two heat-capacity studies for non-terminal alkenes larger than C₃ have been completed; *cis*-hex-2-ene (90MES/TOD) and 2,3-dimethylbut-2-ene (55SCO/FIN). The absence of data for these materials places the determination of group-contribution parameters on a weak basis. See Sec. 4.3.

In Fig. 11 it is apparent that nearly all of the existent studies extend little beyond 298.15 K. The alkenes are excellent candidates for the application of modern differential scanning calorimetric (d.s.c.) methods, which can be used to measure liquid-phase heat capacities to near T_c (89CHI/KNI, 89KNI/ARC).

6.5. Density Data Needs

It is apparent from Table 3 that density measurements for alkenes are numerous. However, measurements at temperatures above 320 K are rare. High-temperature (approaching T_c) measurements would provide a valuable check on the applicability of the corresponding-states

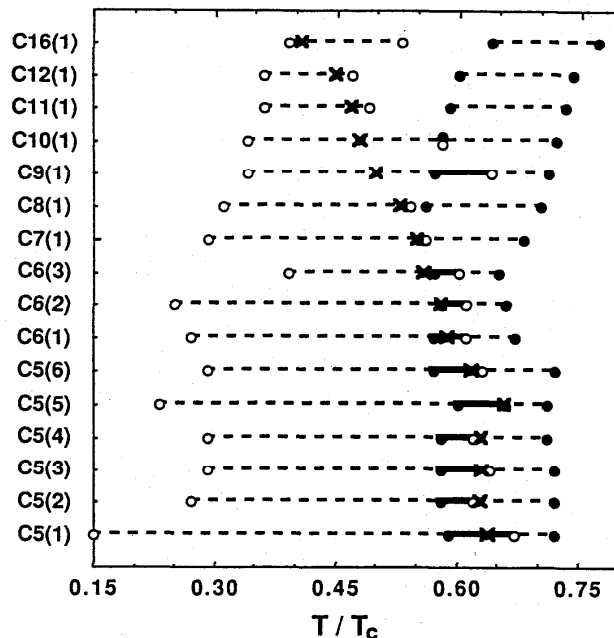


FIG. 11. Liquid-phase heat capacity and vapor-pressure data ranges for the compounds of Table 10. O, Delimits the range of the liquid-phase heat-capacities; ●, delimits the range of the vapor pressures; x, indicates 298.15 K for each compound. The bold lines near $T/T_c = 0.6$ indicate the range of overlap for the data ranges. C₅(1), pent-1-ene; C₅(2), *cis*-pent-2-ene; C₅(3), *trans*-pent-2-ene; C₅(4), 2-methylpent-1-ene; C₅(5), 3-methylpent-1-ene; C₅(6), 2-methylpent-2-ene; C₆(1), hex-1-ene; C₆(2), *cis*-hex-2-ene; C₆(3), 2,3-dimethylbut-2-ene; C₇(1), hept-1-ene; C₈(1), oct-1-ene; C₉(1), non-1-ene; C₁₀(1), dec-1-ene; C₁₁(1), undec-1-ene; C₁₂(1), dodec-1-ene; C₁₆(1), hexadec-1-ene.

equation for these materials in the high-temperature region. These would need to be done in conjunction with reliable critical-property determinations.

6.6. Second Virial Coefficient Data Needs

The excellent accord seen in Table 4 between the calculated and observed second virial coefficients suggests that second virial coefficients can be calculated accurately by corresponding-states methods, providing reliable critical properties are available. It should be noted that reliable critical properties are available for all of the alk-1-enes studied by McGlashan and Wormold (64MCG/WOR). Such good accord cannot be expected, when estimated critical properties are involved, particularly for non-terminal or branched alkenes.

TABLE 1. Critical temperature T_c , critical pressure p_c , critical density ρ_c , and acentric factor ω^a

Compound	T_c/K	Source	p_c/kPa	Source	$\rho_c/(kg\cdot m^{-3})$	Source	ω
PENTENES							
pent-1-ene	464.7	91GUD/ROS	3551	72MOU/KAY	237.7	c	0.237
	465.7	91PEI/YOU	3590	91PEI/YOU	233.4	91PEI/YOU	
	465.1	83WOL/KAY	3553	83WOL/KAY	233	83WOL/KAY	
	463.77	72MOU/KAY			239	91GUD/ROS	
	464.75	60AMB/COX					
	475.55	03VES					
cis-pent-2-ene	474.93	71LEN/REB	3689	71LEN/REB	239.9	c	0.253
trans-pent-2-ene	477	b	3690	b	238.2	c	0.227
2-methylbut-1-ene	471	b	3670	b	241.6	c	0.208
3-methylbut-1-ene	452.7	91PEI/YOU	3530	91PEI/YOU	237.6	c	0.209
					230.0	91PEI/YOU	
2-methylbut-2-ene	470.35	51KIY/SUZ	3415	51KIY/SUZ	241.4	c	0.283
HEXENES							
hex-1-ene	504.2	91GUD/ROS	3206	91GUD/ROS	237.7	c	0.287
	504.0	60AMB/COX			242	91GUD/ROS	
	503.7	91PEI/YOU	3200	91PEI/YOU	232.0	91PEI/YOU	
cis-hex-2-ene	515	b	3300	b	241.0	c	0.278
trans-hex-2-ene	513	b	3300	b	238.5	c	0.280
cis-hex-3-ene	511	b	3300	b	239.2	c	0.279
trans-hex-3-ene	512	b	3300	b	238.1	c	0.277
2-methylpent-1-ene	506	b	3280	b	241.0	c	0.264
3-methylpent-1-ene	495	b	3290	b	239.0	c	0.263
4-methylpent-1-ene	495	b	3290	b	238.0	c	0.257
2-methylpent-2-ene	516	b	3310	b	242.6	c	0.247
3-methyl-cis-pent-2-ene	521	b	3310	b	245.7	c	0.245
3-methyl-trans-pent-2-ene	517	b	3310	b	244.9	c	0.245
4-methyl-cis-pent-2-ene	501	b	3330	b	239.0	c	0.241
4-methyl-trans-pent-2-ene	504	b	3330	b	238.7	c	0.243
2-ethylbut-1-ene	510	b	3280	b	243.9	c	0.261
2,3-dimethylbut-1-ene	501	b	3310	b	243.6	c	0.230
3,3-dimethylbut-1-ene	485	b	3400	b	239.9	c	0.198
2,3-dimethylbut-2-ene	529	b	3330	b	249.9	c	0.216
HEPTENES							
hept-1-ene	537.4	91GUD/ROS	2921	91GUD/ROS	236.6	c	0.342
	537.3	60AMB/COX			244	91GUD/ROS	
cis-hept-2-ene	548	b	2960	b	239.8	c	0.317
trans-hept-2-ene	547	b	2960	b	237.8	c	0.320
cis-hept-3-ene	543	b	2960	b	238.7	c	0.325
trans-hept-3-ene	544	b	2960	b	237.4	c	0.317
2,4-dimethylpent-2-ene	533	b	3000	b	241.5	c	0.263
3-methyl-cis-hex-3-ene	545	b	3060	b	242.0	c	0.320
3-methyl-trans-hex-3-ene	542	b	3060	b	241.3	c	0.322
4,4-dimethylpent-1-ene	520	b	2990	b	240.6	c	0.244
2,4-dimethylpent-1-ene	529	b	2970	b	241.1	c	0.275
4,4-dimethyl-cis-pent-2-ene	534	b	3020	b	245.1	c	0.229
4,4-dimethyl-trans-pent-2-ene	529	b	3020	b	242.7	c	0.220
3-methyl-2-ethylbut-1-ene	536	b	2970	b	245.1	c	0.273
2,3,3-trimethylbut-1-ene	532	b	3010	b	248.3	c	0.214
OCTENES							
oct-1-ene	567.4	91GUD/ROS	2675	91GUD/ROS	235.3	c	0.388
	566.7	60AMB/COX			242	91GUD/ROS	
2-methyl-3-ethylpent-1-ene	558	b	2640	b	244.2	c	0.318
2,2-dimethyl-cis-hex-3-ene	560	b	2730	b	242.6	c	0.273
2,2-dimethyl-trans-hex-3-ene	553	b	2730	b	240.6	c	0.273
2,4,4-trimethylpent-1-ene	556	b	2710	b	245.2	c	0.256
2,4,4-trimethylpent-2-ene	563	b	2740	b	247.0	c	0.243

TABLE 1. Critical temperature T_c , critical pressure p_c , critical density ρ_c , and acentric factor ω^a — Continued

Compound	T_c/K	Source	p_c/kPa	Source	$\rho_c/(kg\cdot m^{-3})$	Source	ω
HIGHER ALK-1-ENES							
non-1-ene	593.7	91GUD/ROS	2450	d	233.7	c	0.435
					241	91GUD/ROS	
dec-1-ene	616.4	91GUD/ROS	2218	91GUD/ROS	232.0	c	0.481
					240	91GUD/ROS	
undec-1-ene	638	e	2070	d	230.0	c	0.527
dodec-1-ene	657.6	91GUD/ROS	1930	91GUD/ROS	228.2	c	0.570
tridec-1-ene	675	e	1760	d	226.7	c	0.606
tetradec-1-ene	692	e	1620	d	225.5	c	0.636
pentadec-1-ene	708	e	1490	d	224.3	c	0.661
hexadec-1-ene	722	e	1370	d	223.0	c	0.693

^aFor compounds with more than one listed value, the first was selected as the reference critical constant for the Cox-equation fit to the vapor pressures.

^bValue was estimated with the group-contribution method of Joback (84JOB).

^cThese values were estimated as described in the text. (See Sec. 2.3.b.)

^dThese values were estimated with a plot of $\ln(\rho_c)$ against carbon number and the measured p_c values for the normal alkenes from Refs. 91GUD/ROS.

^eThese were estimated to be the same as those for the normal alkanes determined experimentally in Ref. 90ANS/GUD.

TABLE 2. Cox equation parameters, temperature ranges, and references for vapor pressures of alkenes^a

Compound	A	B	C	Range/K ^b	Dev ^c	References ^d
PENTENES						
pent-1-ene	2.27398	-2.22095	3.23224	273-335	0.015	49SCO/WAD
				286-304	0.012	50FOR/CAM
<i>cis</i> -pent-2-ene	2.31371	-2.32850	3.32322	275-342	0.006	50SCO/WAD
<i>trans</i> -pent-2-ene	2.24213	-1.87757	2.42550	274-341	0.019	50SCO/WAD
2-methylbut-1-ene	2.22623	-1.85344	2.34988	274-336	0.016	49SCO/WAD
3-methylbut-1-ene	2.22801	-2.11721	3.12559	273-324	0.006	50SCO/WAD
2-methylbut-2-ene	2.32428	-2.29003	3.32064	276-344	0.014	49SCO/WAD
HEXENES						
hex-1-ene	2.35527	-2.24063	2.96550	289-337	0.005	50FOR/CAM
<i>cis</i> -hex-2-ene	2.57865	-3.52828	4.76915	298-342	0.110	56CAM/ROS
<i>trans</i> -hex-2-ene	2.37021	-2.25275	2.84187	292-341	0.015	56CAM/ROS
<i>cis</i> -hex-3-ene	2.35235	-2.18312	2.77968	287-340	0.007	56CAM/ROS
<i>trans</i> -hex-3-ene	2.34309	-2.06211	2.50349	300-341	0.007	56CAM/ROS
2-methylpent-1-ene	2.33746	-2.15965	2.73472	300-336	0.005	56CAM/ROS
3-methylpent-1-ene	2.38928	-2.77455	4.05782	287-328	0.027	56CAM/ROS
4-methylpent-1-ene	2.30327	-2.16715	2.97781	287-327	0.012	56CAM/ROS
2-methylpent-2-ene	2.30384	-1.82956	1.98497	292-341	0.013	56CAM/ROS
3-methyl- <i>cis</i> -pent-2-ene	2.30085	-1.78333	1.87610	290-344	0.010	56CAM/ROS
3-methyl- <i>trans</i> -pent-2-ene	2.28405	-1.77469	1.97631	292-341	0.011	56CAM/ROS
4-methyl- <i>cis</i> -pent-2-ene	2.31171	-2.11660	2.66551	290-330	0.011	56CAM/ROS
4-methyl- <i>trans</i> -pent-2-ene	2.29356	-1.93048	2.29683	292-332	0.011	56CAM/ROS
2-ethylbut-1-ene	2.32440	-1.98465	2.33238	289-338	0.015	56CAM/ROS
2,3-dimethylbut-1-ene	2.26412	-1.86493	2.25861	289-329	0.011	56CAM/ROS
3,3-dimethylbut-1-ene	2.29913	-2.43208	3.37061	291-315	0.018	56CAM/ROS
2,3-dimethylbut-2-ene	2.25445	-1.49430	1.27887	289-347	0.012	56CAM/ROS
				302-346	0.004	55SCO/FIN
HEPTENES						
hept-1-ene	2.42012	-2.19219	2.68682	295-368	0.012	50FOR/CAM
<i>cis</i> -hept-2-ene	2.35368	-1.74767	1.85970	332-372	0.018	70EIS/ORA
<i>trans</i> -hept-2-ene	2.37696	-1.88566	2.07234	331-371	0.009	70EIS/ORA
<i>cis</i> -hept-3-ene	2.36901	-1.86512	2.09361	329-369	0.008	70EIS/ORA
<i>trans</i> -hept-3-ene	2.36093	-1.81666	1.98467	329-369	0.009	70EIS/ORA
2,4-dimethylpent-2-ene	2.36326	-1.95625	2.01980	292-357	0.028	60CAM/ROS
3-methyl- <i>cis</i> -hex-3-ene	2.44297	-2.28418	2.65965	302-368	0.023	60CAM/ROS
3-methyl- <i>trans</i> -hex-3-ene	2.42189	-2.22078	2.64965	300-367	0.012	60CAM/ROS
4,4-dimethylpent-1-ene	2.33088	-2.19135	2.76310	290-346	0.008	60CAM/ROS
2,4-dimethylpent-1-ene	2.35520	-2.09714	2.51745	289-355	0.012	60CAM/ROS
4,4-dimethyl- <i>cis</i> -pent-2-ene	2.31453	-1.97960	2.24165	291-354	0.015	60CAM/ROS
4,4-dimethyl- <i>trans</i> -pent-2-ene	2.29931	-1.72804	1.60871	289-350	0.021	60CAM/ROS
3-methyl-2-ethylbut-1-ene	2.38415	-2.11871	2.36849	290-360	0.010	60CAM/ROS
2,3,3-trimethylbut-1-ene	2.29380	-1.90145	2.08836	288-351	0.014	60CAM/ROS
OCTENES						
oct-1-ene	2.49294	-2.23421	2.55993	318-395	0.007	50FOR/CAM
2-methyl-3-ethylpent-1-ene	2.39909	-2.00415	2.23749	308-383	0.007	60CAM/ROS
2,2-dimethyl- <i>cis</i> -hex-3-ene	2.41397	-2.18706	2.38309	305-379	0.019	60CAM/ROS
2,2-dimethyl- <i>trans</i> -hex-3-ene	2.41812	-2.07272	2.04593	303-374	0.018	60CAM/ROS
2,4,4-trimethylpent-1-ene	2.33539	-1.84581	1.93082	301-375	0.017	60CAM/ROS
2,4,4-trimethylpent-2-ene	2.36322	-1.80757	1.59658	306-378	0.025	60CAM/ROS
HIGHER ALK-1-ENES						
non-1-ene	2.55406	-2.22258	2.38639	340-421	0.009	50FOR/CAM
dec-1-ene	2.61149	-2.20715	2.22656	360-445	0.017	50FOR/CAM
undec-1-ene	2.71104	-2.42496	2.38749	379-467	0.004	50FOR/CAM
dodec-1-ene	2.77553	-2.47981	2.35228	397-488	0.008	50FOR/CAM
tridec-1-ene	2.84230	-2.53546	2.28813	416-506	0.013	55CAM/ROS
tetradec-1-ene	2.82975	-2.27240	1.89478	432-525	0.014	55CAM/ROS
pentadec-1-ene	2.85471	-2.17588	1.67911	447-541	0.012	55CAM/ROS
hexadec-1-ene	2.86441	-2.03715	1.45965	461-558	0.016	54CAM/ROS

^aCox-equation parameters, A, B, and C, are defined by equation (1). The critical properties listed first in Table 1 for each compound were used as the reference temperatures and reference pressures.

^bThe temperature range of the vapor-pressure data used in the fit.

^cThe standard deviation of the experimental values from the fit.

^dThe sources of the vapor-pressure data used in the fit.

TABLE 3. Measured densities ρ , data sources, and deviations from values calculated with corresponding states

T/K	$\rho/(\text{kg}\cdot\text{m}^{-3})^a$	Dev ^b	Reference	T/K	$\rho/(\text{kg}\cdot\text{m}^{-3})^a$	Dev ^b	Reference
<i>pent-1-ene</i>							
293.15	640.50	-0.02	50FOR/CAM	298.2	640.0	-0.09	83WOL/KAY
298.15	635.33	0.01	50FOR/CAM	298.2	635.5	0.05	83WOL/KAY
298.15	635.9	0.10	75DOW/GOO	303.2	631.3	0.22	83WOL/KAY
303.15	630.8	0.16	75DOW/GOO	362.4	556.9	-0.30	83WOL/KAY
153.15	773	-0.10	74KIR	372.6	543.0	-0.30	83WOL/KAY
173.15	755	-0.17	74KIR	383.0	527.8	-0.35	83WOL/KAY
193.15	737	-0.20	74KIR	391.8	514.0	-0.44	83WOL/KAY
213.15	719	-0.16	74KIR	399.6	501.8	-0.38	83WOL/KAY
233.15	700	-0.18	74KIR	406.8	489.8	-0.34	83WOL/KAY
253.15	681	-0.12	74KIR	413.6	477.6	-0.34	83WOL/KAY
273.15	661	-0.10	74KIR	419.6	465.2	-0.53	83WOL/KAY
293.15	641	0.05	74KIR	425.2	453.1	-0.66	83WOL/KAY
313.15	619	0.05	74KIR	430.2	441.9	-0.71	83WOL/KAY
333.15	596	0.09	74KIR	435.0	431.3	-0.54	83WOL/KAY
353.15	572	0.23	74KIR	439.6	420.6	-0.25	83WOL/KAY
373.15	546	0.40	74KIR	444.0	408.9	-0.01	83WOL/KAY
393.15	517	0.56	74KIR	448.2	395.6	0.07	83WOL/KAY
413.15	483	0.61	74KIR	452.2	380.8	0.14	83WOL/KAY
433.15	445	1.56	74KIR	455.8	362.8	-0.34	83WOL/KAY
443.15	418	1.57	74KIR	459.4	341.1	-0.57	83WOL/KAY
293.15	640.6	-0.01	46WIB/GEL	463.0	310.8	0.59	83WOL/KAY
288.15	645.8	-0.03	46WIB/GEL	273.15	663.00	0.21	48DAY/NIC
383.69	541.2	2.38	91PEI/YOU	283.15	652.66	0.22	48DAY/NIC
395.05	521.2	1.97	91PEI/YOU	293.15	642.32	0.26	48DAY/NIC
417.44	479.5	1.61	91PEI/YOU	303.15	631.98	0.35	48DAY/NIC
430.03	454.2	1.96	91PEI/YOU	313.15	621.64	0.48	48DAY/NIC
451.42	389.4	1.56	91PEI/YOU	323.15	611.30	0.67	48DAY/NIC
452.98	386.0	2.38	91PEI/YOU	168.15	751.0	-1.28	41BEN
454.20	381.1	2.54	91PEI/YOU	192.65	735.0	-0.53	41BEN
456.52	371.0	2.96	91PEI/YOU	214.15	718.0	-0.17	41BEN
459.72	344.8	1.18	91PEI/YOU	226.15	711.0	0.43	41BEN
462.06	332.6	3.77	91PEI/YOU	293.15	642.9	0.35	42VAN/MEE
463.40	321.4	6.16	91PEI/YOU	293.15	641.0	0.05	36CAR/WAL
293.15	641.1	0.07	47KAZ/LIB	293.15	641.0	0.05	34SHE/MAY
293.15	641.0	0.05	36SHE/WAL	293.15	642.0	0.21	34SHE/MAY
293.15	647.6	1.08	30DYK/LEW	293.15	641.0	0.05	45GER/VAN
293.15	642.9	0.35	41EWE/HAR	293.15	641.4	0.12	31WIL
293.15	642.3	0.26	50HIL	293.15	640.0	-0.10	49FOE/FEN
298.15	637.2	0.31	50HIL	293.15	640.4	-0.04	50WEI/DEL
303.15	631.9	0.33	50HIL	293.15	641.0	0.05	75ZOT/KIR
293.15	641.0	0.05	36SHE/MOL				
<i>trans-pent-2-ene</i>							
293.15	648.2	-0.02	53ROS/PIT	253.15 c	688.2	0.06	31SEY
298.15	643.1	-0.01	53ROS/PIT	263.15 c	679.1	0.12	31SEY
293.15	648.2	-0.02	75DOW/GOO	273.15 c	669.0	0.08	31SEY
298.15	643.1	-0.01	75DOW/GOO	283.15 c	658.8	0.05	31SEY
303.15	638.0	0.01	75DOW/GOO	293.15 c	648.3	0.00	31SEY
293.15	648.9	0.09	45GER/VAN	303.15 c	637.3	-0.11	31SEY
293.15	648.2	-0.02	41EWE/HAR	313.15 c	626.9	-0.07	31SEY
203.15 c	732.8	-0.13	31SEY	323.15 c	616.2	-0.04	31SEY
213.15 c	724.7	-0.01	31SEY	333.15 c	609.3	0.67	31SEY
223.15 c	715.0	-0.10	31SEY	343.15 c	596.4	0.44	31SEY
233.15 c	706.4	-0.03	31SEY	353.15 c	580.7	-0.21	31SEY
243.15 c	697.4	0.02	31SEY	293.15	650.3	0.30	29SHE/BAL
<i>cis-pent-2-ene</i>							
293.15	656.0	-0.01	75DOW/GOO	293.15	650.3	-0.88	41EWE/HAR
298.15	651.0	0.03	75DOW/GOO	293.15	656.2	0.02	38SHE/LAU
303.15	646.0	0.08	75DOW/GOO	293.15	658.6	0.38	37SHE/MAT
298.15	651.52	0.11	72CUR/FEL	293.15	656.0	-0.01	45GER/VAN
289.65	661.40	0.25	72CUR/FEL	203.15 c	740.4	-0.38	31SEY
274.25	677.20	0.24	72CUR/FEL	213.15 c	731.6	-0.35	31SEY
258.95	692.60	0.26	72CUR/FEL	223.15 c	722.8	-0.29	31SEY
242.95	708.70	0.34	72CUR/FEL	233.15 c	713.9	-0.24	31SEY

TABLE 3. Measured densities ρ , data sources, and deviations from values calculated with corresponding states — Continued

T/K	$\rho/(\text{kg}\cdot\text{m}^{-3})^a$	Dev ^b	Reference	T/K	$\rho/(\text{kg}\cdot\text{m}^{-3})^a$	Dev ^b	Reference	
228.35	722.70	0.36	72CUR/FEL	243.15	c	704.6	-0.21	31SEY
211.9	738.70	0.46	72CUR/FEL	253.15	c	695.1	-0.20	31SEY
197.4	752.60	0.56	72CUR/FEL	263.15	c	685.4	-0.19	31SEY
182.4	767.50	0.75	72CUR/FEL	273.15	c	675.7	-0.14	31SEY
164.55	786.90	1.23	72CUR/FEL	283.15	c	666.1	-0.05	31SEY
144.05	801.40	0.82	72CUR/FEL	293.15	c	656.1	0.00	31SEY
135.15	819.30	2.11	72CUR/FEL	303.15	c	646.0	0.08	31SEY
121.76	830.70	2.11	72CUR/FEL	313.15	c	635.2	0.10	31SEY
293.15	650.5	-0.85	36CAR/WAL	323.15	c	623.9	0.07	31SEY
293.15	655.6	-0.08	53ROS/PIT	333.15	c	612.8	0.12	31SEY
298.15	650.4	-0.06	53ROS/PIT	343.15	c	601.1	0.15	31SEY
293.15	648.1	-1.22	29SHE/BAL	353.15	c	588.6	0.09	31SEY
293.15	655.6	-0.08	51HOF/GRE					
2-methylbut-1-ene								
293.15	650.4	0.00	53ROS/PIT	293.15	650.4	0.00	36SHE/WAL	
298.15	645.1	0.00	53ROS/PIT	293.15	649.0	-0.22	49FOE/FEN	
293.15	650.4	0.00	75DOW/GOO	293.15	650.4	0.00	46SLA	
298.15	645.1	0.00	75DOW/GOO	293.15	650.4	0.00	41EWE/HAR	
303.15	639.6	-0.02	75DOW/GOO	293.15	650.8	0.06	49DER/GRE	
293.15	650.4	0.00	36CAR/WAL	293.15	649.3	-0.17	42VAN/MEE	
293.15	650.6	0.03	45GER/VAN	288.15	650.3	-0.82	36SHE/MOL	
293.15	650.4	0.00	51DES/FID					
3-methylbut-1-ene								
293.15	627.2	-0.02	53ROS/PIT	444.38	357.8	-0.70	91PEI/YOU	
298.15	621.9	0.03	53ROS/PIT	446.91	344.6	-0.30	91PEI/YOU	
293.15	627.2	-0.02	75DOW/GOO	448.64	335.0	0.57	91PEI/YOU	
298.15	621.7	-0.01	75DOW/GOO	288.15	635.0	0.34	45GER/VAN	
303.15	616.1	0.00	75DOW/GOO	288.15	633.8	0.15	33LEE/TUL	
391.00	504.0	1.37	91PEI/YOU	288.15	631.97	-0.14	27NOR/REU	
405.05	475.2	0.72	91PEI/YOU	288.15	632.0	-0.14	36SHE/WAL	
417.05	450.4	0.80	91PEI/YOU	293.15	634.0	1.06	41EWE/HAR	
426.97	424.4	0.46	91PEI/YOU	288.15	632.3	-0.09	36CAR/WAL	
436.87	391.6	-0.14	91PEI/YOU	288.15	632.3	-0.09	36SHE/MOL	
441.68	369.3	-1.05	91PEI/YOU					
2-methylbut-2-ene								
293.15	662.3	-0.01	53ROS/PIT	213.15	730.2	-1.68	31SEY	
298.15	657.0	0.01	53ROS/PIT	223.15	721.6	-1.58	31SEY	
293.15	662.3	-0.01	75DOW/GOO	233.15	713.2	-1.44	31SEY	
298.15	657.0	0.01	75DOW/GOO	243.15	703.4	-1.46	31SEY	
303.15	651.7	0.05	75DOW/GOO	253.15	694.8	-1.30	31SEY	
293.15	662.1	-0.04	73BOU	263.15	686.0	-1.13	31SEY	
293.15	659.6	-0.42	41EWE/HAR	273.15	676.8	-0.99	31SEY	
293.15	662.0	-0.05	36CAR/WAL	283.15	667.2	-0.87	31SEY	
293.15	662.0	-0.05	45GER/VAN	293.15	657.8	-0.69	31SEY	
288.15	667.08	-0.10	27NOR/REU	303.15	646.8	-0.71	31SEY	
298.15	656.94	0.01	27NOR/REU	313.15	635.2	-0.78	31SEY	
293.15	661.9	-0.07	51DES/FID	323.15	623.7	-0.79	31SEY	
293.15	662.0	-0.05	36SHE/WAL	333.15	606.5	-1.67	31SEY	
293.15	660.6	-0.26	49FOE/FEN	343.15	595.0	-1.59	31SEY	
293.15	662.5	0.02	36SHE/MOL	353.15	585.3	-1.12	31SEY	
203.15	738.4	-1.81	31SEY					
hex-1-ene								
293.15	673.17	-0.04	50FOR/CAM	495.11	379.1	4.75	91PEI/YOU	
298.15	668.48	-0.02	50FOR/CAM	498.53	376.8	10.27	91PEI/YOU	
303.15	663.74	-0.01	50FOR/CAM	499.14	358.7	6.35	91PEI/YOU	
293.15	673.6	0.02	46WIB/GEL	500.64	350.4	7.99	91PEI/YOU	
298.15	668.9	0.04	46WIB/GEL	293.15	676.6	0.47	31WIL	
153.15	795	0.07	74KIR	273.15	692.50	0.04	26VAN	
173.15	778	-0.05	74KIR	288.15	678.75	0.08	26VAN	
193.15	762	0.00	74KIR	288.15	684.0	0.86	27BOU	
213.15	745	-0.03	74KIR	293.15	687.3	2.06	40WHI/FEN	
233.15	727	-0.14	74KIR	298.15	668.0	-0.10	68REN/PRA	

TABLE 3. Measured densities ρ , data sources, and deviations from values calculated with corresponding states — Continued

<i>T</i> /K	ρ /(kg·m ⁻³) ^a	Dev ^b	Reference	<i>T</i> /K	ρ /(kg·m ⁻³) ^a	Dev ^b	Reference
253.15	710	-0.05	74KIR	293.15	674.0	0.08	45KOM/UHL
273.15	692	-0.03	74KIR	293.15	674.0	0.08	39CAM/OCO
293.15	673	-0.07	74KIR	293.15	672.9	-0.08	69ROD/HSU
313.15	654	0.00	74KIR	293.15	673.2	-0.04	39GOL/TAY
333.15	635	0.21	74KIR	293.15	675.2	0.26	33WAT/DEK
353.15	614	0.27	74KIR	293.15	674.5	0.16	41VAN/WIB
373.15	592	0.37	74KIR	293.15	683.9	1.55	18BRO/HUM
393.15	568	0.41	74KIR	293.15	673.2	-0.04	50MEA/FOO
413.15	542	0.46	74KIR	298.15	668.4	-0.04	50MEA/FOO
433.15	513	0.50	74KIR	293.15	675.2	0.26	41CAM/EBY2
443.15	497	0.52	74KIR	293.15	673.6	0.02	50WEI/DEL
453.15	480	0.64	74KIR	303.15	664.2	0.06	50WEI/DEL
473.15	438	0.57	74KIR	308.15	659.31	0.06	74LET/MAR
442.54	508.9	2.86	91PEI/YOU	323.15	644.47	0.08	74LET/MAR
456.35	483.1	2.75	91PEI/YOU	298.15	668.80	0.02	75LET
467.80	459.9	2.94	91PEI/YOU	293.15	680.4	1.03	48JEF/VOG
483.51	420.3	3.41	91PEI/YOU	313.15	661.4	1.14	48JEF/VOG
491.27	396.8	4.61	91PEI/YOU	293.15	673.0	-0.07	51DES/FID
298.15	669.01	0.05	86TAR/DIA	293.15	673.2	-0.04	32SCH/BOO
298.15	668.0	-0.10	75WOY	293.15	673.3	-0.02	75ZOT/KIR
<i>cis</i> -hex-2-ene							
293.15	687.20	0.01	56CAM/ROS	293.15	684.49	-0.38	41CAM/EBY2
298.15	682.52	0.02	56CAM/ROS	293.15	686.9	-0.03	51HOF/GRE
303.15	677.76	0.01	56CAM/ROS	298.15	683	0.09	35GRE
298.15	682.0	-0.06	75WOY				
<i>trans</i> -hex-2-ene							
293.15	677.95	-0.01	56CAM/ROS	293.15	678.53	0.07	54POM/FOO
298.15	673.27	-0.01	56CAM/ROS	293.15	678.02	0.00	41CAM/EBY2
303.15	668.47	-0.01	56CAM/ROS	308.15	663.84	0.01	74LET/MAR
298.15	673.1	-0.03	75WOY				
<i>cis</i> -hex-3-ene							
293.15	679.90	-0.02	56CAM/ROS	293.15	679.64	-0.05	41CAM/EBY1
298.15	675.22	-0.01	56CAM/ROS	298.15	674.89	-0.06	41CAM/EBY1
303.15	670.52	0.00	56CAM/ROS	293.15	679.64	-0.05	41CAM/EBY2
293.15	679.5	-0.08	51HOF/GRE	293.15	678.5	-0.22	36CAR/WAL
293.15	678.4	-0.24	38VAN				
<i>trans</i> -hex-3-ene							
293.15	677.11	0.01	56CAM/ROS	293.15	677.9	0.12	38VAN
298.15	672.33	-0.01	56CAM/ROS	293.15	678.5	0.21	36CAR/WAL
303.15	667.47	-0.03	56CAM/ROS	293.15	678.4	0.20	38GIB
293.15	677.18	0.02	54POM/FOO	293.15	677.88	0.12	41CAM/EBY2
293.15	677.88	0.12	41CAM/EBY1	308.15	662.69	-0.03	74LET/MAR
298.15	673.03	0.10	41CAM/EBY1	298.15	671.9	-0.07	75WOY
2-methylpent-1-ene							
293.15	679.87	0.02	56CAM/ROS	293.15	681.7	0.29	40WHI/FEN
298.15	675.05	0.02	56CAM/ROS	293.15	681.7	0.29	46BAR/BUK
303.15	670.20	0.02	56CAM/ROS	293.15	679.85	0.02	53SCH/WIB
293.15	683.1	0.50	31SCH/BOO	298.15	675.09	0.03	53SCH/WIB
293.15	681.7	0.29	32SCH/BOO				
3-methylpent-1-ene							
293.15	667.45	-0.03	56CAM/ROS	293.15	667.5	-0.03	49BOO/HEN
298.15	662.87	0.02	56CAM/ROS	293.15	670.0	0.35	32SCH/BOO
303.15	657.93	0.03	56CAM/ROS				
4-methylpent-1-ene							
293.15	663.70	-0.02	56CAM/ROS	293.15	663.8	-0.01	50MEA/FOO
298.15	658.94	0.00	56CAM/ROS	298.15	658.9	-0.01	50MEA/FOO
303.15	654.00	0.00	56CAM/ROS	293.15	663.9	0.01	49BOO/HEN
302.65	655.6	0.17	74AGA/YUS	293.15	664.7	0.13	41WHI/CAR
322.45	634.5	0.02	74AGA/YUS	293.15	670.7	1.03	30DYK/LEW
347.60	607.5	0.01	74AGA/YUS	293.15	664.6	0.12	32SCH/BOO

TABLE 3. Measured densities ρ , data sources, and deviations from values calculated with corresponding states — Continued

<i>T</i> /K	ρ /(kg·m ⁻³) ^a	Dev ^b	Reference	<i>T</i> /K	ρ /(kg·m ⁻³) ^a	Dev ^b	Reference
2-methylpent-2-ene							
293.15	686.50	-0.01	56CAM/ROS	293.15	690.4	0.55	32SCH/BOO
298.15	681.87	-0.01	56CAM/ROS	273.15	705.1	0.03	23VAN
303.15	676.98	-0.03	56CAM/ROS	288.15	691.45	0.03	23VAN
3-methyl-cis-pent-2-ene							
293.15	697.61	0.00	56CAM/ROS	288.15	702.2	-0.01	22VAN
298.15	693.02	0.01	56CAM/ROS	293.15	698.6	0.14	47HOW/MEA
303.15	688.14	-0.02	56CAM/ROS	298.15	694.2	0.18	47HOW/MEA
293.15	695.6	-0.29	32FLO/BOO				
3-methyl-trans-pent-2-ene							
293.15	693.21	-0.01	56CAM/ROS	288.15	722.0	3.45	22VAN
298.15	688.58	0.00	56CAM/ROS	293.15	694.2	0.13	47HOW/MEA
303.15	683.86	0.00	56CAM/ROS	298.15	689.8	0.18	47HOW/MEA
293.15	694.0	0.11	32FLO/BOO				
4-methyl-cis-pent-2-ene							
293.15	669.18	-0.01	56CAM/ROS	293.15	670.2	0.14	32SCH/BOO
298.15	664.41	-0.01	56CAM/ROS	293.15	670.4	0.17	41WHI/CAR
303.15	659.41	-0.04	56CAM/ROS	298.15	668.5	0.60	35MUL/WAK
4-methyl-trans-pent-2-ene							
293.15	668.62	0.03	56CAM/ROS	293.15	670.9	0.37	32SCH/BOO
298.15	663.80	0.02	56CAM/ROS	293.15	670.6	0.33	10GOR
303.15	658.80	-0.01	56CAM/ROS				
2-ethylbut-1-ene							
293.15	689.58	0.00	56CAM/ROS	293.15	694.03	0.65	21KON
298.15	684.81	0.01	56CAM/ROS	293.15	699.2	1.40	40WHI/FEN
303.15	679.97	0.01	56CAM/ROS	293.15	689.9	0.05	41VAN/WIB
293.15	693.8	0.61	31SCH/BOO	293.15	689.9	0.05	49DER/GRE
293.15	691.4	0.27	32SCH/BOO				
2,3-dimethylbut-1-ene							
293.15	678.10	0.00	56CAM/ROS	293.15	678.01	-0.02	40BRO/HOW
298.15	673.25	0.00	56CAM/ROS	298.15	673.22	0.00	40BRO/HOW
303.15	668.42	0.02	56CAM/ROS	293.15	677.92	-0.03	47HOW/MEA
293.15	682.4	0.63	53HUS/VAN	298.15	673.12	-0.02	47HOW/MEA
293.15	682.7	0.68	31SCH/BOO	293.15	682.5	0.65	41WHI/CAR
293.15	680.3	0.32	32SCH/BOO	293.15	681.0	0.43	33SCH/BOO
3,3-dimethylbut-1-ene							
293.15	653.10	0.03	56CAM/ROS	291.15	654.9	0.00	31FOM/SOC
298.15	647.95	0.01	56CAM/ROS	293.15	651.0	-0.29	33SCH/BOO
303.15	643.02	0.03	56CAM/ROS	293.15	651.9	-0.15	41WIB/GIT
293.15	652.9	0.00	71BAG/MAL	293.15	652.93	0.00	40BRO/HOW
298.15	647.9	0.00	71BAG/MAL	298.15	647.86	-0.01	40BRO/HOW
303.15	642.8	0.00	71BAG/MAL	293.15	653.0	0.01	49BOO/HEN
313.15	632.7	0.03	71BAG/MAL	293.15	651.9	-0.15	41WHI/CAR
2,3-dimethylbut-2-ene							
293.15	708.10	-0.03	56CAM/ROS	293.15	708.1	-0.03	49BOO/HEN
298.15	703.47	-0.03	56CAM/ROS	293.15	708.8	0.07	40BRO/HOW
303.15	699.43	0.05	56CAM/ROS	298.15	704.5	0.12	40BRO/HOW
293.15	708.3	0.00	71BAG/MAL	293.15	707.95	-0.05	47HOW/MEA
298.15	703.7	0.00	71BAG/MAL	298.15	703.36	-0.05	47HOW/MEA
303.15	699.2	0.02	71BAG/MAL	293.15	707.7	-0.08	21VAN
313.15	690.0	0.05	71BAG/MAL	293.15	705.4	-0.41	41WHI/CAR
323.15	680.5	0.06	71BAG/MAL	293.15	708.1	-0.03	33SCH/BOO
293.15	707.6	-0.10	53HUS/VAN	293.15	708.7	0.06	18BRO/HUM
hept-1-ene							
293.15	696.98	-0.02	50FOR/CAM	505.25	439	0.59	74KIR
298.15	692.67	-0.01	50FOR/CAM	298.15	693.3	0.08	75WOY

TABLE 3. Measured densities ρ , data sources, and deviations from values calculated with corresponding states — Continued

<i>T/K</i>	$\rho/(\text{kg}\cdot\text{m}^{-3})^a$	<i>Dev</i> ^b	Reference	<i>T/K</i>	$\rho/(\text{kg}\cdot\text{m}^{-3})^a$	<i>Dev</i> ^b	Reference
303.15	688.15	-0.02	50FOR/CAM	283.15	706.9	0.15	48LAG/MCM
173.15	796	0.17	74KIR	293.15	699.5	0.34	48LAG/MCM
193.15	780	0.09	74KIR	303.15	691.0	0.39	48LAG/MCM
213.15	764	0.05	74KIR	298.15	692.9	0.02	46WIB/GEL
233.15	748	0.05	74KIR	293.15	697.0	-0.02	36CAR/WAL
253.15	731	-0.03	74KIR	298.15	694.0	0.18	41IRW/HEN
273.15	714	-0.06	74KIR	293.15	697.0	-0.02	34SHE/MAY
293.15	697	-0.02	74KIR	293.15	697.0	-0.02	36SHE/MOL
313.15	679	-0.04	74KIR	293.15	697.2	0.01	34SHE/MAY
333.15	661	0.03	74KIR	293.15	697.7	0.08	31WIL
353.15	642	0.07	74KIR	293.15	700.4	0.47	39CAM/OCO
373.15	623	0.25	74KIR	293.15	699.3	0.31	33SOD/BOO
393.15	602	0.29	74KIR	293.15	700.0	0.41	45GRI
413.15	580	0.39	74KIR	293.15	699.3	0.31	39GOL/TAY
433.15	556	0.44	74KIR	293.15	700.0	0.41	58HIL/HAY
443.15	544	0.63	74KIR	293.15	697.1	-0.01	41VAN/WIB
453.15	531	0.76	74KIR	293.15	700.96	0.55	41CAM/EBY2
473.15	500	0.57	74KIR	293.15	694.5	-0.38	43CAM/YOU
493.15	465	0.64	74KIR	293.15	697.1	-0.01	44APP/DOB
<i>cis</i> -hept-2-ene							
293.15	707.1	0.01	53ROS/PIT ^d	293.15	708	0.14	53ROS/PIT
298.15	702.8	0.01	53ROS/PIT ^d	298.15	704	0.18	53ROS/PIT
298.15	703.8	0.16	75WOY	298.15	705	0.33	35GRE
<i>trans</i> -hept-2-ene							
293.15	701.2	0.00	53ROS/PIT	298.15	696.1	-0.12	75WOY
298.15	696.9	0.00	53ROS/PIT	293.15	700.9	-0.04	73EIS/KUD
<i>cis</i> -hept-3-ene							
293.15	702.8	-0.02	53ROS/PIT	293.15	705.3	0.34	73EIS/KUD
298.15	698.5	-0.01	53ROS/PIT				
<i>trans</i> -hept-3-ene							
293.15	698.1	0.00	53ROS/PIT	298.15	693.2	-0.08	75WOY
298.15	693.8	0.00	53ROS/PIT	293.15	699.1	0.14	73EIS/KUD
3-methyl- <i>cis</i> -hex-3-ene							
293.15	712.87	0.03	60CAM/ROS	303.15	704.13	0.04	60CAM/ROS
298.15	707.95	-0.04	60CAM/ROS				
3-methyl- <i>trans</i> -hex-3-ene							
293.15	709.65	0.02	60CAM/ROS	303.15	700.94	0.04	60CAM/ROS
298.15	705.06	-0.01	60CAM/ROS				
2,4-dimethylpent-1-ene							
293.15	694.10	0.01	60CAM/ROS	293.15	694.3	0.04	49BOO/HEN
298.15	689.66	0.02	60CAM/ROS	293.15	693.7	-0.05	33SOD/BOO
303.15	685.17	0.03	60CAM/ROS				
4,4-dimethylpent-1-ene							
293.15	682.49	0.00	60CAM/ROS	298.15	688.3	1.54	35MUL/WAK
298.15	678.04	0.02	60CAM/ROS	293.15	682.7	0.03	49BOO/HEN
303.15	673.51	0.03	60CAM/ROS	293.15	680.2	-0.33	58HIL/HAY
293.15	682.7	0.03	33WHI/HOM				
2,4-dimethylpent-2-ene							
293.15	694.92	-0.01	60CAM/ROS	293.15	695.2	0.03	42WIB/VAN
298.15	690.52	0.00	60CAM/ROS	293.15	695.5	0.07	41VAN/WIB
303.15	685.91	-0.02	60CAM/ROS	293.15	694.7	-0.04	31DEG
293.15	695.10	0.02	42WIB/VAN	293.15	695.0	0.00	49BOO/HEN
4,4-dimethyl- <i>cis</i> -pent-2-ene							
293.15	699.43	-0.02	60CAM/ROS	303.15	690.61	0.00	60CAM/ROS
298.15	695.10	0.00	60CAM/ROS				

TABLE 3. Measured densities ρ , data sources, and deviations from values calculated with corresponding states — Continued

T/K	$\rho/(\text{kg}\cdot\text{m}^{-3})^a$	Dev ^b	Reference	T/K	$\rho/(\text{kg}\cdot\text{m}^{-3})^a$	Dev ^b	Reference
4,4-dimethyl-trans-pent-2-ene							
293.15	688.85	0.04	60CAM/ROS	293.15	688.4	-0.03	40CRA/MIL
298.15	684.30	0.02	60CAM/ROS	293.15	688.1	-0.07	40CRA/MIL
303.15	679.54	-0.01	60CAM/ROS				
3-methyl-2-ethylbut-1-ene							
293.15	708.78	0.01	60CAM/ROS	303.15	699.68	0.00	60CAM/ROS
298.15	704.29	0.01	60CAM/ROS	293.15	718.6	1.40	33SOD/BOO
2,3,3-trimethylbut-1-ene							
293.15	704.66	-0.03	60CAM/ROS	298.15	700.54	0.03	40BRO/HOW
298.15	700.24	-0.02	60CAM/ROS	293.15	704.8	-0.01	49BOO/HEN
303.15	695.73	-0.01	60CAM/ROS	273.15	723.5	0.12	22CHA/LEJ
293.15	705.01	0.02	40BRO/HOW	288.15	710.1	0.10	22CHA/LEJ
oct-1-ene							
293.15	714.92	-0.02	50FOR/CAM	283.15	723.8	0.08	48LAG/MCM
298.15	710.85	-0.02	50FOR/CAM	293.15	718.3	0.45	48LAG/MCM
303.15	706.58	-0.03	50FOR/CAM	303.15	710.0	0.45	48LAG/MCM
173.15	815	1.04	74KIR	293.15	715.1	0.01	46WIB/GEL
193.15	799	0.87	74KIR	298.15	711.0	0.01	46WIB/GEL
213.15	782	0.59	74KIR	293.15	715.8	0.10	31WIL
233.15	765	0.35	74KIR	293.15	715.8	0.10	48JEF/VOG
253.15	748	0.14	74KIR	312.85	700.1	0.20	48JEF/VOG
273.15	732	0.11	74KIR	333.25	682.6	0.20	48JEF/VOG
293.15	715	-0.01	74KIR	360.15	661.1	0.58	48JEF/VOG
313.15	698	-0.07	74KIR	303.15	709.0	0.31	79PUG/MUK
333.15	681	-0.05	74KIR	313.15	700.5	0.29	79PUG/MUK
353.15	663	-0.10	74KIR	323.15	692.1	0.31	79PUG/MUK
373.15	645	-0.04	74KIR	333.15	683.2	0.27	79PUG/MUK
393.15	626	-0.01	74KIR	343.15	674.5	0.29	79PUG/MUK
413.15	606	0.02	74KIR	353.15	665.6	0.29	79PUG/MUK
433.15	584	-0.09	74KIR	363.15	656.8	0.34	79PUG/MUK
443.15	574	0.12	74KIR	293.15	714.86	-0.03	54POM/FOO
453.15	563	0.23	74KIR	293.15	715.0	-0.01	41HEN/CHA
473.15	539	0.40	74KIR	293.15	716.0	0.13	43HEN/GRE
493.15	513	0.73	74KIR	293.15	715.0	-0.01	43CLE
511.45	482	0.30	74KIR	293.15	715.1	0.01	49BOO/HEN
293.15	716.95	0.26	41CAM/EBY2	293.15	724.0	1.25	18BRO/HUM
293.15	715.2	0.02	45KOM/UHL	298.15	711.8	0.12	88DYM/MAL
293.15	717.5	0.34	49FOE/FEN	323.15	690.9	0.13	88DYM/MAL
293.15	714.7	-0.05	69ROD/HSU	348.15	669.2	0.16	88DYM/MAL
293.15	715.5	0.06	39GOL/TAY	373.15	646.6	0.21	88DYM/MAL
293.15	710.94	-0.58	56WEB	293.15	718.1	0.42	32WAT/TEN
293.15	716.1	0.15	41VAN/WIB	293.15	715.0	-0.01	42BOO
2,2-dimethyl-cis-hex-3-ene							
293.15	712.51	0.00	60CAM/ROS	293.15	718.65	0.87	44HEN/MAT
298.15	708.35	0.01	60CAM/ROS	293.15	718.6	0.86	49BOO/HEN
303.15	704.16	0.01	60CAM/ROS				
2,2-dimethyl-trans-hex-3-ene							
293.15	703.82	0.04	60CAM/ROS	303.15	694.83	-0.04	60CAM/ROS
298.15	699.31	0.00	60CAM/ROS	293.15	704.0	0.07	49BOO/HEN
2-methyl-3-ethylpent-1-ene							
293.15	724.68	-0.01	60CAM/ROS	303.15	716.4	0.03	60CAM/ROS
298.15	720.60	0.02	60CAM/ROS				
2,4,4-trimethylpent-1-ene							
293.15	714.97	-0.02	60CAM/ROS	298.15	710.81	-0.01	52POM
298.15	710.89	0.00	60CAM/ROS	293.15	715.00	-0.02	47HOW/MEA
303.15	706.54	-0.01	60CAM/ROS	298.15	710.76	-0.02	47HOW/MEA
293.15	715.1	-0.01	36CAR/WAL	293.15	715.1	-0.01	32TON/PIC
293.15	715.12	0.00	52POM	293.15	714.9	-0.03	49BOO/HEN

TABLE 3. Measured densities ρ , data sources, and deviations from values calculated with corresponding states — Continued

T/K	ρ /(kg·m ⁻³) ^a	Dev ^b	Reference	T/K	ρ /(kg·m ⁻³) ^a	Dev ^b	Reference
2,4,4-trimethylpent-2-ene							
293.15	721.23	0.03	60CAM/ROS	293.15	721.77	0.11	52POM
298.15	716.94	0.02	60CAM/ROS	298.15	717.55	0.10	52POM
303.15	712.59	0.00	60CAM/ROS	293.15	721.24	0.03	47HOW/MEA
293.15	721.1	0.01	36CAR/WAL	298.15	717.00	0.02	47HOW/MEA
293.15	722.3	0.18	41VAN/WIB	293.15	721.1	0.01	32TON/PIC
non-1-ene							
293.15	729.22	-0.01	50FOR/CAM	413.15	626	-0.23	74KIR
298.15	725.31	-0.01	50FOR/CAM	433.15	607	-0.16	74KIR
303.15	721.34	-0.02	50FOR/CAM	443.15	597	-0.13	74KIR
193.15	808	0.69	74KIR	453.15	587	-0.06	74KIR
213.15	792	0.46	74KIR	473.15	565	-0.06	74KIR
233.15	776	0.25	74KIR	283.15	741.1	0.56	48LAG/MCM
253.15	761	0.20	74KIR	293.15	733.0	0.51	48LAG/MCM
273.15	745	0.06	74KIR	303.15	725.2	0.51	48LAG/MCM
293.15	729	-0.04	74KIR	293.15	729.3	0.00	46WIB/GEL
313.15	713	-0.09	74KIR	298.15	725.3	-0.02	46WIB/GEL
333.15	696	-0.22	74KIR	293.15	731.5	0.30	31WIL
353.15	679	-0.29	74KIR	293.15	815.5	11.82	55HIL/SIM
373.15	662	-0.27	74KIR	288.15	754.7	2.94	15CLA/ADA
393.15	645	-0.15	74KIR	293.15	729.1	-0.03	49TIL/PES
dec-1-ene							
293.15	740.81	0.02	50FOR/CAM	433.15	625	-0.17	74KIR
298.15	736.93	-0.01	50FOR/CAM	443.15	615	-0.27	74KIR
303.15	733.04	-0.03	50FOR/CAM	453.15	607	0.00	74KIR
293.15	740.8	0.01	46WIB/GEL	473.15	588	0.20	74KIR
298.15	736.9	-0.01	46WIB/GEL	283.15	751.0	0.40	48LAG/MCM
213.15	803	0.72	74KIR	293.15	743.5	0.38	48LAG/MCM
233.15	787	0.44	74KIR	303.15	735.9	0.36	48LAG/MCM
253.15	771	0.19	74KIR	293.15	742.1	0.19	48JEF/VOG
273.15	756	0.09	74KIR	312.95	726.9	0.14	48JEF/VOG
293.15	741	0.04	74KIR	332.85	712.3	0.23	48JEF/VOG
313.15	725	-0.11	74KIR	359.45	691.6	0.29	48JEF/VOG
333.15	709	-0.20	74KIR	293.15	741.8	0.15	34WAR/FUL
353.15	693	-0.24	74KIR	293.15	741.0	0.04	50MEA/FOO
373.15	677	-0.21	74KIR	298.15	737.1	0.01	50MEA/FOO
393.15	660	-0.25	74KIR	293.15	743.7	0.41	53HIL/HAY
413.15	643	-0.19	74KIR	293.15	741.0	0.04	49TIL/PES
undec-1-ene							
293.15	750.32	0.04	50FOR/CAM	283.15	759.4	0.31	48LAG/MCM
298.15	746.55	0.01	50FOR/CAM	293.15	752.3	0.30	48LAG/MCM
303.15	742.76	-0.02	50FOR/CAM	303.15	744.7	0.24	48LAG/MCM
293.15	750.6	0.08	49TIL/PES				
dodec-1-ene							
293.15	758.36	0.02	50FOR/CAM	313.75	745.0	0.13	48JEF/VOG
298.15	754.74	-0.01	50FOR/CAM	332.95	731.5	0.14	48JEF/VOG
303.15	751.0	-0.04	50FOR/CAM	359.65	712.1	0.13	48JEF/VOG
293.15	758.9	0.09	46WIB/GEL	293.15	760.0	0.24	38EVA
298.15	755.3	0.07	46WIB/GEL	323.15	738.4	0.13	38EVA
293.15	759.3	0.14	49TIL/PES	293.15	767.2	1.19	56PET/SER
293.15	760.1	0.25	48JEF/VOG				
tridec-1-ene							
293.15	765.27	0.04	55CAM/ROS	293.15	766.6	0.21	49TIL/PES
298.15	761.68	0.00	55CAM/ROS	273.15	779.8	0.22	46SCH/HER
303.15	758.01	-0.04	55CAM/ROS	293.15	765.6	0.08	46SCH/HER
293.15	773.9	1.17	48LAG/MCM	310.93	752.8	-0.04	46SCH/HER
298.15	767.0	0.70	48LAG/MCM	333.15	736.6	-0.19	46SCH/HER
303.15	759.6	0.17	48LAG/MCM	372.04	708.1	-0.35	46SCH/HER
273.15	785.6	0.97	38KOZ/REI	293.15	773.2	1.08	56PET/SER
298.15	767.0	0.70	38KOZ/REI				

TABLE 3. Measured densities ρ , data sources, and deviations from values calculated with corresponding states — Continued

<i>T</i> /K	ρ /(kg·m ⁻³) ^a	Dev ^b	Reference	<i>T</i> /K	ρ /(kg·m ⁻³) ^a	Dev ^b	Reference
tetradec-1-ene							
293.15	771.27	0.01	55CAM/ROS	314.05	758.1	0.06	48JEF/VOG
298.15	767.67	-0.04	55CAM/ROS	334.55	744.0	-0.01	48JEF/VOG
303.15	764.16	-0.08	55CAM/ROS	359.95	727.1	0.03	48JEF/VOG
293.15	772.6	0.18	48JEF/VOG	293.15	772.5	0.17	56PET/SER
pentadec-1-ene							
293.15	776.41	0.06	55CAM/ROS	298.15	775.1	0.30	38KOZ/REI
298.15	772.90	0.01	55CAM/ROS	273.15	789.8	0.19	46SCH/HER
303.15	769.39	-0.04	55CAM/ROS	293.15	775.7	-0.03	46SCH/HER
293.15	786.7	1.39	48LAG/MCM	310.93	763.3	-0.19	46SCH/HER
298.15	780.0	0.93	48LAG/MCM	333.15	747.8	-0.36	46SCH/HER
303.15	773.1	0.45	48LAG/MCM	372.04	720.9	-0.54	46SCH/HER
273.15	792.1	0.49	38KOZ/REI	293.15	775.5	-0.05	56PET/SER
hexadec-1-ene							
293.15	781.12	0.04	54CAM/FOR	288.15	784.2	0.04	(83)KRA
298.15	777.59	-0.03	54CAM/FOR	310.25	768.9	-0.19	(83)KRA
303.15	774.09	-0.08	54CAM/FOR	288.35	789.3	0.71	(60)MEN
293.15	781.2	0.05	46WIB/GEL	287.75	794.9	1.37	06EYK
298.15	777.7	-0.01	46WIB/GEL	352.95	739.4	-0.54	06EYK
293.15	782.4	0.20	48JEF/VOG	293.15	781.0	0.02	24GAU/ALT
314.55	767.7	0.00	48JEF/VOG	293.15	786.8	0.76	24SEY/HUG
333.95	754.5	-0.14	48JEF/VOG	298.15	779.0	0.15	29COR
358.85	737.8	-0.24	48JEF/VOG	293.15	784.8	0.51	34WAR/FUL
293.15	782.5	0.21	50MUM/PHI	293.15	783.8	0.38	37LAN/STE
298.15	779.2	0.18	50MUM/PHI	288.15	785.77	0.24	38SCH
293.15	782.5	0.21	29WAT/VAN	293.15	782.33	0.19	38SCH
277.15	791.5	0.12	(83)KRA	298.15	778.89	0.14	38SCH
288.15	783.9	0.00	(83)KRA	293.15	782.7	0.24	38EVA
310.25	768.6	-0.23	(83)KRA	323.15	761.5	-0.11	38EVA
277.15	791.7	0.15	(83)KRA	293.15	780.5	-0.04	56PET/SER

^aThe measured density from the literature cited.

^bDev is the percentage deviation of the literature value from that calculated with equation (2) and the critical properties listed in Table 1.

^cDensities by Seyer (31SEY) for *cis* and *trans* pent-2-ene are relative values only. The original values were derived by assuming the value at 293.15 K by Sherrill *et al.* (29SHE/BAL) to be correct. The values listed in this table were derived by assuming the value at 293.15 K calculated with Eq. (2) is correct.

^dThe densities for *cis*-hept-2-ene published with the results for API Project 44 (53ROS/PIT) were later revised within that project. The revised values are listed in Ref. 90TRC.

TABLE 4. Measured second virial coefficients, data sources, and deviations from values calculated with corresponding states

<i>T</i> /K	$10^6 B$ (m ³ /mol) ^a	Dev ^b	Reference	<i>T</i> /K	$10^6 B$ (m ³ /mol) ^a	Dev ^b	Reference
pent-1-ene							
283.95	-1276	3.7	49SCO/WAD	353.3	-712	-2.1	64MCG/WOR
298.15	-1143	5.1	49SCO/WAD	363.9	-662	-2.6	64MCG/WOR
303.1	-1099	5.2	49SCO/WAD	374.0	-628	-1.6	64MCG/WOR
308.0	-982	-2.2	64MCG/WOR	383.2	-585	-3.1	64MCG/WOR
315.3	-930	-2.1	64MCG/WOR	393.8	-552	-2.6	64MCG/WOR
324.1	-870	-2.2	64MCG/WOR	403.4	-519	-3.2	64MCG/WOR
334.1	-810	-2.2	64MCG/WOR	410.4	-486	-5.7	64MCG/WOR
344.3	-756	-2.1	64MCG/WOR				
2-methylbut-1-ene							
277.96	-1258	-1.3	49SCO/WAD	304.3	-1117	9.7	49SCO/WAD
298.15	-1163	8.7	49SCO/WAD				
2-methylbut-2-ene							
289.89	-1382	3.7	49SCO/WAD	311.71	-1134	2.6	49SCO/WAD
298.15	-1278	3.2	49SCO/WAD				
hex-1-ene							
313.8	-1493	0.2	64MCG/WOR	373.1	-947	-2.0	64MCG/WOR
325.7	-1340	-0.9	64MCG/WOR	383.4	-886	-2.1	64MCG/WOR
333.7	-1262	-0.8	64MCG/WOR	392.6	-845	-1.2	64MCG/WOR
342.6	-1194	0.3	64MCG/WOR	403.2	-779	-3.0	64MCG/WOR
353.8	-1087	-1.1	64MCG/WOR	410.3	-763	-0.9	64MCG/WOR
364.3	-1009	-1.5	64MCG/WOR				
hept-1-ene							
333.8	-1847	0.4	64MCG/WOR	374.2	-1370	0.1	64MCG/WOR
338.2	-1809	-1.1	64MCG/WOR	383.8	-1288	-0.2	64MCG/WOR
343.6	-1760	-2.6	64MCG/WOR	393.3	-1196	1.1	64MCG/WOR
353.8	-1614	-1.8	64MCG/WOR	403.3	-1120	0.8	64MCG/WOR
364.0	-1482	-0.7	64MCG/WOR	411.4	-1069	1.1	64MCG/WOR
oct-1-ene							
358.8	-2162	-1.6	64MCG/WOR	383.8	-1818	-2.7	64MCG/WOR
363.2	-2100	-2.1	64MCG/WOR	389.9	-1728	-1.8	64MCG/WOR
368.1	-2000	-0.9	64MCG/WOR	395.4	-1666	-1.8	64MCG/WOR
374.5	-1941	-2.6	64MCG/WOR	403.7	-1552	-0.2	64MCG/WOR
375.3	-1914	-1.8	64MCG/WOR	411.6	-1465	0.6	64MCG/WOR
383.3	-1823	-2.6	64MCG/WOR				

^aThe measured density from the literature cited.

^bDev is the percentage deviation of the literature value from that calculated with the corresponding-states equation of Pitzer and Curl (57PIT/CUR) and the critical properties listed in Table 1.

TABLE 5. Comparison of measured enthalpies of vaporization with those calculated with the Cox and Clapeyron equations

T/K	$\Delta_f H_m(\text{lit})/RK^a$	$\Delta_f H_m(\text{Cox})/RK^b$	Diff ^c	int/ext ^d	K ^e	Reference
pent-1-ene						
283.95	3157 ± 3	3158 ± 8	-1	int		49SCO/WAD
298.15	3064 ± 3	3064 ± 12	0	int		49SCO/WAD
303.11	3030 ± 2	3030 ± 13	0	int		49SCO/WAD
310.93	2966 ± 4	2975 ± 16	-9	int		63CUF/KOZ
310.92	2970 ± 4	2975 ± 16	-5	int		63CUF/KOZ
327.57	2849 ± 4	2851 ± 22	-2	int		63CUF/KOZ
344.25	2706 ± 4	2716 ± 29	-10	ext	9	63CUF/KOZ
344.25	2709 ± 4	2716 ± 29	-7	ext	9	63CUF/KOZ
344.24	2709 ± 4	2716 ± 29	-7	ext	9	63CUF/KOZ
360.91	2565 ± 4	2569 ± 37	-4	ext	26	63CUF/KOZ
377.59	2390 ± 4	2409 ± 46	-19	ext	43	63CUF/KOZ
377.58	2396 ± 4	2409 ± 46	-13	ext	43	63CUF/KOZ
394.26	2211 ± 4	2232 ± 57	-21	ext	59	63CUF/KOZ
410.93	1996 ± 4	2032 ± 68	-36	ext	76	63CUF/KOZ
410.93	1988 ± 4	2032 ± 68	-44	ext	76	63CUF/KOZ
2-methylbut-1-ene						
277.96	3249 ± 1	3246 ± 7	3	int		49SCO/WAD
298.15	3110 ± 4	3117 ± 11	-7	int		49SCO/WAD
304.30	3067 ± 2	3074 ± 13	-7	int		49SCO/WAD
2-methylbut-2-ene						
289.89	3309 ± 1	3310 ± 9	-1	int		49SCO/WAD
298.15	3255 ± 1	3255 ± 11	0	int		49SCO/WAD
311.71	3164 ± 1	3160 ± 14	4	int		49SCO/WAD
2,3-dimethylbut-2-ene						
292.13	3953 ± 1	3946 ± 4	7	int		55SCO/FIN
307.85	3845 ± 1	3849 ± 6	-4	int		55SCO/FIN
325.77	3717 ± 1	3727 ± 10	-10	int		55SCO/FIN
346.34	3564 ± 2	3569 ± 16	-5	int		55SCO/FIN
oct-1-ene						
298.15	4843 ± 15	4852 ± 6	-9	ext	-20	82SVO/CHA
313.15	4753 ± 15	4739 ± 4	14	ext	-5	82SVO/CHA
328.15	4645 ± 14	4626 ± 5	19	int		82SVO/CHA
343.15	4525 ± 14	4510 ± 7	15	int		82SVO/CHA
358.15	4398 ± 14	4392 ± 11	6	int		82SVO/CHA
368.15	4306 ± 13	4311 ± 13	-5	int		82SVO/CHA
298.15	4843 ± 24	4852 ± 6	-9	ext	-20	77MAN/SEL
298.15	4800 ± ?	4852 ± 6	-52	ext	-20	81CHI/HYM
298.15	4960 ± ?	4852 ± 6	108	ext	-20	81CHI/HYM
dec-1-ene						
298.15	6065 ± 24	6012 ± 63	53	ext	-62	77MAN/SEL
dodec-1-ene						
298.15	7310 ± 24	7300 ± 28	10	ext	-99	77MAN/SEL
hexadec-1-ene						
298.15	9652 ± 24	9460 ± 750	192	ext	-163	77MAN/SEL

^aMeasured enthalpy of vaporization reported in the literature.

^bEnthalpy of vaporization derived from measured vapor pressures and equation (3).

^cThe literature value minus the value derived with equation (3).

^d"int" indicates that the temperature of the literature enthalpy of vaporization was within the range of the vapor-pressure data. "ext" indicates that an extrapolation of the vapor-pressure data was required.

^eThe magnitude of the extrapolation in Kelvin.

TABLE 6. Enthalpies of vaporization at 298.15 K used for calculation of enthalpies of formation for the gas state ($R = 8.31451 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$)

Compound	$\Delta_f H_m / \text{RK}$	Source ^a
PENTENES		
pent-1-ene	3064 ± 12	Cox fit
<i>cis</i> -pent-2-ene	3231 ± 10	Cox fit
<i>trans</i> -pent-2-ene	3219 ± 10	Cox fit
2-methylbut-1-ene	3117 ± 11	Cox fit
3-methylbut-1-ene	2859 ± 14	Cox fit
2-methylbut-2-ene	3255 ± 11	Cox fit
HEXENES		
hex-1-ene	3681 ± 6	Cox fit
<i>cis</i> -hex-2-ene	3872 ± 32	Cox fit
<i>trans</i> -hex-2-ene	3800 ± 6	Cox fit
<i>cis</i> -hex-3-ene	3756 ± 6	Cox fit
<i>trans</i> -hex-3-ene	3794 ± 6	Cox fit
2-methylpent-1-ene	3666 ± 7	Cox fit
3-methylpent-1-ene	3442 ± 9	Cox fit
4-methylpent-1-ene	3453 ± 8	Cox fit
2-methylpent-2-ene	3801 ± 6	Cox fit
3-methyl- <i>cis</i> -pent-2-ene	3860 ± 5	Cox fit
3-methyl- <i>trans</i> -pent-2-ene	3771 ± 6	Cox fit
4-methyl- <i>cis</i> -pent-2-ene	3546 ± 7	Cox fit
4-methyl- <i>trans</i> -pent-2-ene	3604 ± 7	Cox fit
2-ethylbut-1-ene	3744 ± 6	Cox fit
2,3-dimethylbut-1-ene	3509 ± 7	Cox fit
3,3-dimethylbut-1-ene	3201 ± 10	Cox fit
2,3-dimethylbut-2-ene	3910 ± 5	Cox fit
HEPTENES		
hept-1-ene	4269 ± 5	Cox fit
<i>cis</i> -hept-2-ene	4361 ± 18	Cox fit
<i>trans</i> -hept-2-ene	4362 ± 11	Cox fit
<i>cis</i> -hept-3-ene	4307 ± 8	Cox fit
<i>trans</i> -hept-3-ene	4311 ± 10	Cox fit
2,4-dimethylpent-2-ene	4112 ± 5	Cox fit
3-methyl- <i>cis</i> -hex-3-ene	4367 ± 5	Cox fit
3-methyl- <i>trans</i> -hex-3-ene	4294 ± 4	Cox fit
4,4-dimethylpent-1-ene	3744 ± 6	Cox fit
2,4-dimethylpent-1-ene	3973 ± 5	Cox fit
4,4-dimethyl- <i>cis</i> -pent-2-ene	3916 ± 5	Cox fit
4,4-dimethyl- <i>trans</i> -pent-2-ene	3946 ± 6	Cox fit
3-methyl-2-ethylbut-1-ene	4131 ± 5	Cox fit
2,3,3-trimethylbut-1-ene	3860 ± 5	Cox fit
OCTENES		
oct-1-ene	4852 ± 6	Cox fit
2-methyl-3-ethylpent-1-ene	4483 ± 4	Cox fit
2,2-dimethyl- <i>cis</i> -hex-3-ene	4433 ± 5	Cox fit
2,2-dimethyl- <i>trans</i> -hex-3-ene	4454 ± 4	Cox fit
2,4,4-trimethylpent-1-ene	4281 ± 5	Cox fit
2,4,4-trimethylpent-2-ene	4478 ± 6	Cox fit
HIGHER ALKENES		
dec-1-ene	6065 ± 24	77MAN/SEL
2,2,5,5-tetramethyl- <i>trans</i> -hex-3-ene	5052 ± 30	79FUC/PEA2
dodec-1-ene	7310 ± 24	77MAN/SEL
hexadec-1-ene	9652 ± 24	77MAN/SEL

^a"Cox fit" indicates that the value was derived with Eq. (1) and the Clapeyron equation (Eq. 3).

TABLE 7. Enthalpies of combustion for the liquid phase with data sources, and derived enthalpies of formation for the liquid and gas phases.
 $T = 298.15 \text{ K}$ and $p^\circ = 101.325 \text{ kPa}$.^{a,b}

Compound	$\Delta_c H_m^\circ(\text{liquid})$	Reference	$\Delta_f H_m^\circ(\text{liquid})$	$\Delta_f H_m^\circ(\text{gas})$
PENTENES				
pent-1-ene	-3349.72 ± 0.58	79GOO/SMI	-46.98 ± 0.84	-21.50 ± 0.87
<i>cis</i> -pent-2-ene	-3343.21 ± 0.54	79GOO/SMI	-53.49 ± 0.82	-26.63 ± 0.83
	-3336.70 ± 0.30	46COO/MUL	-60.00 ± 0.68	
<i>trans</i> -pent-2-ene	-3338.71 ± 0.70	79GOO/SMI	-57.99 ± 0.93	-31.23 ± 0.94
	-3335.90 ± 0.40	46COO/MUL	-60.80 ± 0.73	
2-methylbut-1-ene	-3335.74 ± 0.80	79GOO/SMI	-60.96 ± 1.01	-35.57 ± 1.02
3-methylbut-1-ene	-3345.10 ± 0.54	79GOO/SMI	-51.60 ± 0.82	-27.83 ± 0.85
2-methylbut-2-ene	-3328.62 ± 1.26	79GOO/SMI	-68.08 ± 1.40	-41.02 ± 1.41
HEXENES				
hex-1-ene	-4005.72 ± 1.30	56BAR	-70.32 ± 1.46	-39.71 ± 1.46
<i>cis</i> -hex-2-ene	-3998.2 ± 1.3	revised c	-77.8 ± 1.5	-45.6 ± 1.6
	-3994.21 ± 1.34	56BAR	-81.83 ± 1.50	
<i>trans</i> -hex-2-ene	-3992.58 ± 1.55	56BAR	-83.46 ± 1.69	-51.86 ± 1.69
<i>cis</i> -hex-3-ene	-3999.15 ± 1.30	56BAR	-76.89 ± 1.46	-45.66 ± 1.46
<i>trans</i> -hex-3-ene	-3992.04 ± 1.30	56BAR	-84.00 ± 1.46	-52.45 ± 1.46
2-methylpent-1-ene	-3988.15 ± 1.26	56BAR	-87.89 ± 1.42	-57.41 ± 1.43
3-methylpent-1-ene	-3999.95 ± 1.51	56BAR	-76.09 ± 1.65	-47.47 ± 1.66
4-methylpent-1-ene	-3998.06 ± 1.76	56BAR	-77.98 ± 1.88	-49.27 ± 1.88
2-methylpent-2-ene	-3979.57 ± 1.42	56BAR	-96.47 ± 1.57	-64.87 ± 1.58
3-methyl- <i>cis</i> -pent-2-ene	-3983.75 ± 1.46	56BAR	-92.29 ± 1.61	-60.20 ± 1.61
3-methyl- <i>trans</i> -pent-2-ene	-3983.59 ± 1.21	56BAR	-92.45 ± 1.39	-61.10 ± 1.39
4-methyl- <i>cis</i> -pent-2-ene	-3991.08 ± 1.17	56BAR	-84.96 ± 1.35	-55.48 ± 1.35
4-methyl- <i>trans</i> -pent-2-ene	-3986.56 ± 1.34	56BAR	-89.48 ± 1.50	-59.51 ± 1.50
2-ethylbut-1-ene	-3991.03 ± 1.46	56BAR	-85.01 ± 1.61	-53.88 ± 1.61
2,3-dimethylbut-1-ene	-3982.50 ± 1.67	56BAR	-93.54 ± 1.80	-64.36 ± 1.81
3,3-dimethylbut-1-ene	-3989.78 ± 1.51	56BAR	-86.26 ± 1.65	-59.65 ± 1.66
2,3-dimethylbut-2-ene	-3975.68 ± 1.42	56BAR	-100.36 ± 1.57	-67.85 ± 1.58
HEPTENES				
hept-1-ene	-4657.00 ± 0.80	76GOO	-98.38 ± 1.08	-62.89 ± 1.08
	-4658.34 ± 1.17	61ROC/ROS	-97.04 ± 1.38	
	-4651.00 ± 0.80	46COO/MUL	-104.38 ± 1.08	
<i>cis</i> -hept-2-ene	-4650.22 ± 0.79	76GOO	-105.16 ± 1.07	-68.90 ± 1.08
<i>trans</i> -hept-2-ene	-4645.83 ± 0.75	76GOO	-109.55 ± 1.04	-73.28 ± 1.04
<i>cis</i> -hept-3-ene	-4651.06 ± 0.67	76GOO	-104.32 ± 0.99	-68.51 ± 0.99
<i>trans</i> -hept-3-ene	-4646.04 ± 0.92	76GOO	-109.34 ± 1.17	-73.50 ± 1.17
5-methylhex-1-ene	-4655.40 ± 0.50	46COO/MUL	-99.98 ± 0.88	d
2,4-dimethylpent-2-ene	-4632.25 ± 0.84	61ROC/ROS	-123.13 ± 1.11	-88.94 ± 1.11
3-methyl- <i>cis</i> -hex-3-ene	-4639.38 ± 0.89	61ROC/ROS	-116.00 ± 1.14	-79.69 ± 1.15
3-methyl- <i>trans</i> -hex-3-ene	-4642.59 ± 0.84	61ROC/ROS	-112.79 ± 1.11	-77.09 ± 1.11
4,4-dimethylpent-1-ene	-4644.78 ± 1.68	61ROC/ROS	-110.60 ± 1.83	-79.47 ± 1.83
2,4-dimethylpent-1-ene	-4638.36 ± 1.16	61ROC/ROS	-117.02 ± 1.37	-83.99 ± 1.37
4,4-dimethyl- <i>cis</i> -pent-2-ene	-4650.05 ± 1.21	61ROC/ROS	-105.33 ± 1.41	-72.77 ± 1.41
4,4-dimethyl- <i>trans</i> -pent-2-ene	-4633.60 ± 0.84	61ROC/ROS	-121.78 ± 1.11	-88.97 ± 1.11

TABLE 7. Enthalpies of combustion for the liquid phase with data sources, and derived enthalpies of formation for the liquid and ideal-gas phases.
 $T = 298.15 \text{ K}$ and $p^\circ = 101.325 \text{ kPa}$.^{a,b} — Continued

Compound	$\Delta_c H_m^\circ(\text{liquid})$	Reference	$\Delta_f H_m^\circ(\text{liquid})$	$\Delta_f H_m^\circ(\text{gas})$
3-methyl-2-ethylbut-1-ene	-4641.29 ± 1.35	61ROC/ROS	-114.09 ± 1.53	-79.74 ± 1.54
2,3,3-trimethylbut-1-ene	-4637.66 ± 1.16	61ROC/ROS	-117.72 ± 1.37	-85.63 ± 1.37
OCTENES				
oct-1-ene	-5312.93 ± 1.13	61ROC/ROS	-121.79 ± 1.37	-81.45 ± 1.37
2-methyl-3-ethylpent-1-ene	-5296.99 ± 0.74	61ROC/ROS	-137.73 ± 1.07	-100.46 ± 1.08
2,2-dimethyl- <i>cis</i> -hex-3-ene	-5308.30 ± 2.39	61ROC/ROS	-126.42 ± 2.51	-89.56 ± 2.51
	-5298.37 ± 3.10	73YAT/MCD	-136.35 ± 3.19	
2,2-dimethyl- <i>trans</i> -hex-3-ene	-5289.76 ± 1.28	61ROC/ROS	-144.96 ± 1.49	-107.96 ± 1.49
	-5276.94 ± 3.85	73YAT/MCD	-157.78 ± 3.93	
2,4,4-trimethylpent-1-ene	-5289.07 ± 0.69	61ROC/ROS	-145.65 ± 1.04	-110.06 ± 1.04
2,4,4-trimethylpent-2-ene	-5292.31 ± 1.75	61ROC/ROS	-142.41 ± 1.92	-105.18 ± 1.92
2,5-dimethyl- <i>cis</i> -hex-3-ene	-5283.68 ± 3.68	73YAT/MCD	-151.04 ± 3.76	d
2,5-dimethyl- <i>trans</i> -hex-3-ene	-5275.48 ± 2.93	73YAT/MCD	-159.24 ± 3.03	d
DECENES				
dec-1-ene	-6619.59 ± 1.84	61ROC/ROS	-173.81 ± 2.03	-123.38 ± 2.03
2,2,5,5-tetramethyl- <i>cis</i> -hex-3-ene	-6629.85 ± 3.33	61ROC/ROS	-163.55 ± 3.44	d
2,2,5,5-tetramethyl- <i>trans</i> -hex-3-ene	-6585.76 ± 4.67	61ROC/ROS	-207.64 ± 4.75	-165.64 ± 4.76
HIGHER ALK-1-ENES				
dodec-1-ene	-7925.90 ± 1.30	76STR	-226.18 ± 1.61	-165.40 ± 1.61
hexadec-1-ene	-10539.00 ± 2.00	76STR	-330.44 ± 2.28	-249.59 ± 2.28^c
	-10546.01 ± 3.05	60LOE/ROS	-323.43 ± 3.24	
	-10540.20 ± 1.85	55FRA/PRO	-329.24 ± 2.15	

^aAll listed values are in $\text{kJ}\cdot\text{mol}^{-1}$. All uncertainties are the "uncertainty interval" as defined in 56ROS.

^bThe first value listed for each compound was selected as the most reliable, and was used in all further calculations.

^cThis value was revised in accord with the experimental equilibria (see Sec. 3.7.) and the enthalpy-of-hydrogenation and hydration results (see Sec. 4.3.).

^dGas-phase properties cannot be calculated for this compound because no enthalpies of vaporization or vapor pressures have been measured.

^eThis value was calculated from the average of the enthalpy-of-combustion values reported in Refs. 76STR and 55FRA/PRO.

TABLE 8. Molar thermodynamic functions at vapor-saturation pressure ($R = 8.31451 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$)

$\frac{T}{\text{K}}$	$\frac{C_{\text{sat,m}}}{R}$	$\frac{\Delta_f^{\circ} S_m^{\circ}}{R}$	$\frac{\Delta_f^{\circ} H_m^{\circ}}{RT}$	$\frac{T}{\text{K}}$	$\frac{C_{\text{sat,m}}}{R}$	$\frac{\Delta_f^{\circ} S_m^{\circ}}{R}$	$\frac{\Delta_f^{\circ} H_m^{\circ}}{RT}$
pent-1-ene							
cr							
10.00	0.20	0.07	0.05	70.00	6.68	5.17	3.18
20.00	1.26	0.49	0.36	80.00	7.34	6.10	3.66
30.00	2.66	1.26	0.89	90.00	7.94	7.00	4.10
40.00	3.93	2.21	1.50	100.00	8.48	7.87	4.51
50.00	5.00	3.20	2.09	108.03	8.91	8.54	4.82
60.00	5.91	4.20	2.66				
liquid							
135.61	16.00	17.33	12.58	260.00	17.74	28.04	14.48
140.00	15.99	17.84	12.69	280.00	18.33	29.38	14.74
160.00	16.03	19.98	13.10	298.15 a	18.92	30.55	14.97
180.00	16.17	21.87	13.44	300.00 a	18.98	30.67	15.00
200.00	16.43	23.59	13.72	320.00 a	19.71	31.92	15.27
220.00	16.78	25.17	13.98	340.00 a	20.51	33.13	15.55
240.00	17.22	26.65	14.23	350.00 a	20.93	33.73	15.70
3-methylbut-1-ene							
cr							
10.00	0.21	0.07	0.05	70.00	6.17	4.89	2.97
20.00	1.25	0.50	0.36	80.00	6.84	5.76	3.42
30.00	2.55	1.25	0.88	90.00	7.48	6.60	3.83
40.00	3.69	2.15	1.44	100.00	8.12	7.42	4.23
50.00	4.64	3.08	1.99	104.72	8.43	7.81	4.41
60.00	5.45	3.99	2.50				
liquid							
104.72	14.65	13.96	10.57	260.00	17.43	27.99	13.59
120.00	14.66	15.95	11.09	280.00	18.10	29.31	13.89
140.00	14.81	18.22	11.61	298.15	18.77	30.46	14.17
160.00	15.06	20.21	12.02	300.00 a	18.84	30.58	14.20
180.00	15.40	22.01	12.38	320.00 a	19.66	31.82	14.51
200.00	15.81	23.65	12.70	340.00 a	20.55	33.04	14.84
220.00	16.29	25.18	13.00	350.00 a	21.02	33.64	15.01
240.00	16.83	26.62	13.30				
2-methylbut-2-ene							
cr							
10.00	0.18	0.06	0.05	70.00	6.70	4.91	3.05
20.00	1.14	0.44	0.32	80.00	7.51	5.85	3.56
30.00	2.46	1.15	0.81	90.00	8.26	6.78	4.04
40.00	3.70	2.03	1.38	100.00	8.97	7.69	4.50
50.00	4.81	2.98	1.96	120.00	10.29	9.44	5.35
60.00	5.80	3.94	2.52	139.42	11.59	11.08	6.13
liquid							
139.42	15.90	17.63	12.69	260.00	17.31	27.76	14.37
140.00	15.90	17.70	12.70	280.00	17.84	29.06	14.60
160.00	15.88	19.82	13.10	298.15	18.38	30.20	14.81
180.00	15.99	21.70	13.41	300.00	18.44	30.31	14.83
200.00	16.19	23.39	13.68	320.00 a	19.12	31.52	15.08
220.00	16.48	24.95	13.92	340.00 a	19.87	32.71	15.34
240.00	16.85	26.40	14.15	350.00 a	20.27	33.29	15.48

TABLE 8. Molar thermodynamic functions at vapor-saturation pressure ($R = 8.31451 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$) — Continued

$\frac{T}{\text{K}}$	$\frac{C_{\text{sat,m}}}{R}$	$\frac{\Delta_f^{\circ} S_m^{\circ}}{R}$	$\frac{\Delta_f^{\circ} H_m^{\circ}}{RT}$	$\frac{T}{\text{K}}$	$\frac{C_{\text{sat,m}}}{R}$	$\frac{\Delta_f^{\circ} S_m^{\circ}}{R}$	$\frac{\Delta_f^{\circ} H_m^{\circ}}{RT}$	
hex-1-ene								
cr								
10.00	0.21	0.07	0.05	70.00	7.28	5.39	3.35	
20.00	1.26	0.50	0.36	80.00	8.10	6.42	3.89	
30.00	2.68	1.27	0.90	90.00	8.84	7.41	4.40	
40.00	4.07	2.23	1.52	100.00	9.52	8.38	4.88	
50.00	5.29	3.28	2.15	120.00	10.75	10.23	5.76	
60.00	6.35	4.34	2.77	133.38	11.52	11.40	6.30	
liquid								
133.38	18.55	19.83	14.73	260.00	20.67	32.58	16.91	
140.00	18.54	20.73	14.91	280.00	21.37	34.14	17.20	
160.00	18.58	23.21	15.36	298.15	22.06	35.50	17.48	
180.00	18.76	25.40	15.73	300.00	22.13	35.64	17.51	
200.00	19.07	27.40	16.04	320.00	a	22.97	37.09	17.82
220.00	19.50	29.23	16.34	340.00	a	23.87	38.51	18.15
240.00	20.04	30.95	16.62	350.00	a	24.34	39.21	18.32
250.00	20.34	31.77	16.77					
cis-hex-2-ene								
cr								
10.00	0.19	0.06	0.05	70.00	7.39	5.34	3.34	
20.00	1.20	0.46	0.34	80.00	8.28	6.39	3.91	
30.00	2.64	1.21	0.86	90.00	9.08	7.41	4.44	
40.00	4.06	2.17	1.49	100.00	9.82	8.40	4.94	
50.00	5.30	3.21	2.13	120.00	11.25	10.32	5.87	
60.00	6.41	4.28	2.75	132.04	12.19	11.44	6.40	
liquid								
132.04	18.51	19.52	14.49	260.00	20.12	32.26	16.65	
140.00	18.45	20.60	14.72	280.00	20.79	33.78	16.92	
160.00	18.40	23.06	15.18	298.15	21.46	35.10	17.18	
180.00	18.50	25.24	15.54	300.00	21.53	35.24	17.21	
200.00	18.73	27.20	15.85	320.00	a	22.33	36.65	17.50
220.00	19.07	29.00	16.13	340.00	a	23.21	38.03	17.81
240.00	19.54	30.67	16.39	350.00	a	23.68	38.71	17.97
250.00	19.82	31.48	16.52					
2,3-dimethylbut-2-ene								
cr(II)								
10.00	0.18	0.06	0.04	90.00	10.05	7.86	4.78	
20.00	1.18	0.44	0.32	100.00	10.90	8.97	5.35	
30.00	2.68	1.20	0.86	120.00	12.35	11.09	6.40	
40.00	4.23	2.18	1.51	140.00	13.61	13.09	7.34	
50.00	5.66	3.28	2.20	160.00	14.91	14.99	8.20	
60.00	6.94	4.43	2.88	180.00	16.47	16.83	9.03	
70.00	8.09	5.59	3.54	196.86	18.14	18.38	9.74	
80.00	9.12	6.73	4.18					
cr(I)								
196.86	18.12	20.53	11.90	198.96	18.12	20.73	11.96	
liquid								
198.96	18.48	24.62	15.86	298.15	21.02	32.50	17.09	
200.00	18.49	24.72	15.87	300.00	21.09	32.63	17.12	
220.00	18.81	26.50	16.13	320.00	21.83	34.01	17.39	
240.00	19.25	28.15	16.37	340.00	a	22.64	35.36	17.67
250.00	19.50	28.94	16.49	360.00	a	23.52	36.68	17.97
260.00	19.78	29.71	16.61	380.00	a	24.46	37.98	18.29
280.00	20.40	31.20	16.86	400.00	a	25.47	39.26	18.62

TABLE 8. Molar thermodynamic functions at vapor-saturation pressure ($R = 8.31451 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$) – Continued

$\frac{T}{\text{K}}$	$\frac{C_{\text{sat,m}}}{R}$	$\frac{\Delta_f^\circ S_m^\circ}{R}$	$\frac{\Delta_f^\circ H_m^\circ}{RT}$	$\frac{T}{\text{K}}$	$\frac{C_{\text{sat,m}}}{R}$	$\frac{\Delta_f^\circ S_m^\circ}{R}$	$\frac{\Delta_f^\circ H_m^\circ}{RT}$
hept-1-ene							
cr(II)							
10.00	0.22	0.06	0.04	70.00	8.01	5.74	3.60
20.00	1.30	0.51	0.38	80.00	8.97	6.88	4.21
30.00	2.80	1.31	0.93	90.00	9.82	7.98	4.79
40.00	4.32	2.33	1.59	100.00	10.60	9.06	5.33
50.00	5.70	3.44	2.28	120.00	12.03	11.12	6.33
60.00	6.93	4.59	2.95	137.00	13.17	12.79	7.11
cr(I)							
137.00	13.15	13.01	7.33	150.00	14.02	14.24	7.87
140.00	13.35	13.30	7.46	154.31	14.30	14.64	8.05
liquid							
154.31	21.81	24.31	17.71	260.00	23.94	36.02	19.67
160.00	21.80	25.10	17.86	280.00	24.71	37.82	20.01
180.00	21.92	27.67	18.30	298.15	25.48	39.39	20.32
200.00	22.23	29.99	18.68	300.00	25.57	39.55	20.35
220.00	22.68	32.13	19.02	320.00	a	41.23	20.70
240.00	23.26	34.13	19.35	340.00	a	42.87	21.08
250.00	23.59	35.09	19.51	350.00	a	43.68	21.27
oct-1-ene							
cr							
10.00	0.28	0.09	0.07	80.00	9.96	7.93	4.79
20.00	1.59	0.65	0.47	90.00	10.87	9.16	5.42
30.00	3.30	1.61	1.13	100.00	11.69	10.35	6.00
40.00	4.99	2.80	1.89	120.00	13.18	12.61	7.08
50.00	6.49	4.08	2.66	140.00	14.57	14.75	8.05
60.00	7.80	5.38	3.41	160.00	15.97	16.79	8.95
70.00	8.95	6.67	4.12	171.48	16.79	17.92	9.45
liquid							
171.48	25.60	28.66	20.19	280.00	28.19	41.55	22.60
180.00	25.54	29.90	20.44	298.15	29.03	43.35	22.96
200.00	25.63	32.59	20.96	300.00	29.12	43.53	23.00
220.00	26.01	35.05	21.40	320.00	a	45.44	23.42
240.00	26.60	37.34	21.80	340.00	a	47.30	23.84
260.00	27.35	39.50	22.20	360.00	a	49.12	24.29
non-1-ene							
cr(II)							
10.00	0.25	0.08	0.06	90.00	11.88	9.44	5.69
20.00	1.49	0.60	0.44	100.00	12.86	10.74	6.36
30.00	3.22	1.52	1.07	120.00	14.61	13.25	7.59
40.00	5.02	2.69	1.83	140.00	16.18	15.62	8.71
50.00	6.72	4.00	2.64	160.00	17.73	17.88	9.74
60.00	8.25	5.36	3.45	180.00	19.36	20.06	10.72
70.00	9.61	6.74	4.24	182.00	19.53	20.27	10.81
80.00	10.81	8.10	4.99				
cr(I)							
182.00	20.07	20.66	11.20	191.92	21.19	21.75	11.69
190.00	20.97	21.54	11.59				

TABLE 8. Molar thermodynamic functions at vapor-saturation pressure ($R = 8.31451 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$) — Continued

$\frac{T}{\text{K}}$	$\frac{C_{\text{sat,m}}}{R}$	$\frac{\Delta_f^{\circ} S_m^{\circ}}{R}$	$\frac{\Delta_f^{\circ} H_m^{\circ}}{RT}$	$\frac{T}{\text{K}}$	$\frac{C_{\text{sat,m}}}{R}$	$\frac{\Delta_f^{\circ} S_m^{\circ}}{R}$	$\frac{\Delta_f^{\circ} H_m^{\circ}}{RT}$	
liquid								
191.92	29.37	33.89	23.82	320.00	33.71	49.56	26.63	
200.00	29.26	35.09	24.04	340.00	34.83	51.63	27.08	
220.00	29.41	37.89	24.52	360.00	35.96	53.66	27.54	
240.00	29.95	40.47	24.95	380.00	37.10	55.63	28.02	
260.00	30.71	42.89	25.36	400.00	a	38.26	57.56	28.50
280.00	31.62	45.20	25.77	420.00	a	39.43	59.46	28.99
298.15	32.53	47.21	26.16	440.00	a	40.62	61.32	29.49
300.00	32.62	47.42	26.20	450.00	a	41.22	62.24	29.75
dec-1-ene								
cr(II)								
10.00	0.30	0.10	0.08	90.00	12.98	10.47	6.27	
20.00	1.74	0.70	0.51	100.00	14.03	11.90	6.99	
30.00	3.64	1.76	1.23	120.00	15.96	14.63	8.33	
40.00	5.58	3.07	2.08	140.00	17.74	17.22	9.55	
50.00	7.41	4.52	2.96	160.00	19.56	19.71	10.69	
60.00	9.05	6.02	3.84	180.00	21.70	22.13	11.78	
70.00	10.50	7.52	4.69	198.30	24.78	24.35	12.81	
80.00	11.80	9.01	5.50					
cr(I)								
198.30	33.34	29.17	17.63	206.93	35.36	30.63	18.33	
200.00	33.74	29.46	17.77					
liquid								
206.93	33.36	38.66	26.36	340.00	38.62	56.00	29.81	
220.00	33.14	40.69	26.77	360.00	a	39.90	58.25	30.33
240.00	33.47	43.58	27.31	380.00	a	41.26	60.44	30.87
260.00	34.21	46.29	27.81	400.00	a	42.68	62.59	31.42
280.00	35.18	48.86	28.30	420.00	a	44.18	64.71	32.00
298.15	36.16	51.10	28.75	440.00	a	45.74	66.80	32.59
300.00	36.26	51.32	28.79	450.00	a	46.55	67.84	32.89
320.00	37.40	53.70	29.29					
undec-1-ene								
cr(II)								
10.00	0.29	0.10	0.07	90.00	14.10	11.23	6.78	
20.00	1.77	0.69	0.51	100.00	15.24	12.78	7.57	
30.00	3.85	1.79	1.27	120.00	17.28	15.74	9.02	
40.00	6.01	3.20	2.19	140.00	19.14	18.54	10.33	
50.00	8.02	4.76	3.16	160.00	21.06	21.22	11.55	
60.00	9.83	6.39	4.12	180.00	23.12	23.82	12.72	
70.00	11.43	8.02	5.05	200.00	25.56	26.38	13.88	
80.00	12.84	9.64	5.94	217.30	28.41	28.61	14.92	
cr(I)								
217.30	39.31	33.71	20.02	224.01	41.92	34.95	20.63	
220.00	40.36	34.20	20.26					
liquid								
224.01	37.23	44.07	29.76	300.00	39.81	55.15	31.85	
240.00	37.11	46.62	30.25	320.00	a	41.10	57.76	32.39
260.00	37.74	49.62	30.79	340.00	a	42.55	60.29	32.94
280.00	38.68	52.45	31.32	350.00	a	43.33	61.54	33.23

TABLE 8. Molar thermodynamic functions at vapor-saturation pressure ($R = 8.31451 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$) — Continued

$\frac{T}{\text{K}}$	$\frac{C_{\text{sat,m}}}{R}$	$\frac{\Delta_f^\circ S_m^\circ}{R}$	$\frac{\Delta_f^\circ H_m^\circ}{RT}$	$\frac{T}{\text{K}}$	$\frac{C_{\text{sat,m}}}{R}$	$\frac{\Delta_f^\circ S_m^\circ}{R}$	$\frac{\Delta_f^\circ H_m^\circ}{RT}$
dodec-1-ene ^b							
cr(II)							
10.00	0.38	0.13	0.10	90.00	15.44	12.42	7.43
20.00	2.09	0.87	0.63	100.00	16.71	14.12	8.30
30.00	4.27	2.12	1.47	120.00	19.07	17.37	9.90
40.00	6.54	3.66	2.46	140.00	21.24	20.48	11.36
50.00	8.73	5.35	3.49	160.00	23.49	23.46	12.74
60.00	10.73	7.12	4.54	180.00	26.20	26.37	14.08
70.00	12.50	8.91	5.55	200.00	30.36	29.32	15.47
80.00	14.06	10.69	6.52	212.90	36.46	31.38	16.53
cr(I)							
212.90	43.14	33.96	19.11	230.00	44.95	37.21	20.82
220.00	41.21	35.31	19.82	237.95	49.00	38.81	21.70
liquid							
237.95	41.18	48.87	31.76	320.00 a	44.86	61.43	34.51
240.00	41.13	49.22	31.84	340.00 a	46.39	64.20	35.16
260.00	41.41	52.52	32.56	360.00 a	48.10	66.89	35.83
280.00	42.33	55.62	33.22	380.00 a	49.98	69.54	36.53
298.15	43.38	58.31	33.81	400.00 a	52.05	72.16	37.25
300.00	43.50	58.58	33.87				
hexadec-1-ene ^b							
cr(III)							
10.00	0.42	0.14	0.10	90.00	19.64	15.33	9.30
20.00	2.37	0.96	0.70	100.00	21.30	17.49	10.42
30.00	5.10	2.43	1.70	120.00	24.38	21.65	12.49
40.00	8.06	4.30	2.92	140.00	27.20	25.62	14.39
50.00	10.87	6.40	4.23	160.00	29.88	29.42	16.16
60.00	13.52	8.62	5.56	180.00	32.87	33.11	17.84
70.00	15.83	10.88	6.87	200.00	36.55	36.76	19.52
80.00	17.83	13.13	8.11	217.70	46.75	40.13	21.17
cr(II)							
217.70	41.08	40.13	21.17	240.00	49.48	44.44	23.32
220.00	41.58	40.56	21.38	249.20	64.10	46.53	24.51
230.00	44.35	42.46	22.31				
cr(I)							
249.20	69.22	48.39	26.37	270.00	83.68	54.09	29.83
260.00	68.85	51.26	28.09	277.40	103.72	56.61	31.51
liquid							
277.40	57.49	69.66	44.56	380.00	66.11	88.84	49.05
280.00	57.56	70.20	44.68	400.00 a	68.41	92.29	49.96
298.15	58.44	73.84	45.49	420.00 a	70.88	95.69	50.90
300.00	58.57	74.20	45.57	440.00 a	73.52	99.05	51.87
320.00	60.19	78.03	46.43	460.00 a	76.33	102.38	52.87
340.00	61.99	81.73	47.29	480.00 a	79.30	105.69	53.91
360.00	63.97	85.33	48.17	500.00 a	82.45	108.99	54.99

^aValues at this temperature were calculated with graphically extrapolated heat capacities.

^bThere is evidence that dodec-1-ene and hexadec-1-ene retain end-to-end disorder to 0 K in the crystal phase. The magnitude of the error in the crystal-phase entropies is unknown, while the liquid-phase entropies are probably low by $0.69\cdot R$ (i.e., $R\cdot\ln 2$). See Sec. 5.2.

TABLE 9. Enthalpies of vaporization obtained from the Cox and Clapeyron equations

<i>T</i> /K	$\Delta_i^{\#}H_m/RK$	<i>T</i> /K	$\Delta_i^{\#}H_m/RK$	<i>T</i> /K	$\Delta_i^{\#}H_m/RK$	<i>T</i> /K	$\Delta_i^{\#}H_m/RK$			
pent-1-ene										
240.00	a	3420 ± 3	280.00	3183 ± 8	300.00	3052 ± 12	340.00	a	2751 ± 27	
260.00	a	3305 ± 4	298.15	3064 ± 12	320.00	2908 ± 19	350.00	a	2667 ± 32	
<i>cis</i> -pent-2-ene										
240.00	a	3600 ± 2	280.00	3352 ± 6	300.00	3218 ± 11	340.00		2918 ± 24	
260.00	a	3478 ± 4	298.15	3231 ± 10	320.00	3074 ± 17	350.00	a	2835 ± 29	
<i>trans</i> -pent-2-ene										
240.00	a	3554 ± 4	280.00	3333 ± 6	300.00	3207 ± 11	340.00		2907 ± 24	
260.00	a	3448 ± 4	298.15	3219 ± 10	320.00	3066 ± 17	350.00	a	2821 ± 29	
2-methylbut-1-ene										
240.00	a	3457 ± 3	280.00	3234 ± 7	300.00	3104 ± 12	340.00	a	2794 ± 26	
260.00	a	3350 ± 4	298.15	3117 ± 11	320.00	2958 ± 18	350.00	a	2704 ± 31	
3-methylbut-1-ene										
240.00	a	3209 ± 3	280.00	2978 ± 9	300.00	2846 ± 14	340.00	a	2537 ± 31	
260.00	a	3098 ± 5	298.15	2859 ± 14	320.00	2700 ± 22	350.00	a	2449 ± 36	
2-methylbut-2-ene										
240.00	a	3618 ± 4	280.00	3374 ± 7	300.00	3242 ± 11	340.00		2944 ± 25	
260.00	a	3499 ± 4	298.15	3255 ± 11	320.00	3100 ± 17	350.00	a	2861 ± 30	
hex-1-ene										
250.00	a	3991 ± 5	280.00	a	3800 ± 4	300.00	3668 ± 7	340.00	a	3380 ± 17
260.00	a	3928 ± 3	298.15		3681 ± 6	320.00	3529 ± 11	350.00	a	3301 ± 21
<i>cis</i> -hex-2-ene										
250.00	a	4333 ± 300	280.00	a	4043 ± 64	300.00	3855 ± 30	340.00		3487 ± 31
260.00	a	4235 ± 187	298.15		3872 ± 32	320.00	3670 ± 18	350.00	a	3395 ± 48
2,3-dimethylbut-2-ene										
250.00	a	4175 ± 9	298.15		3910 ± 5	340.00	3620 ± 14	400.00	a	3051 ± 40
260.00	a	4124 ± 6	300.00		3899 ± 5	360.00	a	3452 ± 21		
280.00	a	4016 ± 4	320.00		3768 ± 9	380.00	a	3263 ± 30		
hept-1-ene										
250.00	a	4598 ± 25	298.15		4269 ± 5	340.00	3970 ± 11	380.00	a	3649 ± 25
260.00	a	4529 ± 16	300.00		4256 ± 5	350.00	3894 ± 14	400.00	a	3468 ± 34
280.00	a	4393 ± 7	320.00		4116 ± 7	360.00	3815 ± 17	420.00	a	3271 ± 45
oct-1-ene										
260.00	a	5143 ± 26	300.00	a	4838 ± 6	360.00	4377 ± 11	420.00	a	3847 ± 34
280.00	a	4989 ± 12	320.00		4688 ± 5	380.00	4211 ± 17	440.00	a	3642 ± 45
298.15	a	4852 ± 6	340.00		4535 ± 7	400.00	a	4036 ± 25		
non-1-ene										
298.15	a	5434 ± 14	340.00		5094 ± 5	400.00	4586 ± 18	450.00	a	4093 ± 40
300.00	a	5419 ± 13	360.00		4931 ± 7	420.00	4399 ± 25	460.00	a	3983 ± 46
320.00	a	5256 ± 6	380.00		4762 ± 12	440.00	a	4199 ± 35		
dec-1-ene										
298.15	a	6012 ± 63	360.00		5471 ± 8	440.00	4726 ± 28	500.00	a	4028 ± 64
300.00	a	5996 ± 59	380.00		5296 ± 9	450.00	a	4621 ± 33		
320.00	a	5819 ± 30	400.00		5115 ± 13	460.00	a	4513 ± 38		
340.00	a	5644 ± 13	420.00		4926 ± 19	480.00	a	4281 ± 50		
undec-1-ene										
298.15	a	6674 ± 10	350.00	a	6138 ± 3	420.00	5446 ± 14	500.00	a	4555 ± 52
300.00	a	6654 ± 10	360.00	a	6039 ± 4	440.00	5240 ± 21	520.00	a	4291 ± 67
320.00	a	6443 ± 6	380.00		5842 ± 5	460.00	5025 ± 29			
340.00	a	6238 ± 4	400.00		5646 ± 9	480.00	a	4797 ± 40		
dodec-1-ene										
298.15	a	7300 ± 28	360.00	a	6595 ± 5	440.00	5747 ± 16	520.00	a	4802 ± 57
300.00	a	7277 ± 27	380.00	a	6382 ± 4	460.00	5528 ± 23	540.00	a	4523 ± 72
320.00	a	7042 ± 16	400.00		6171 ± 6	480.00	5300 ± 32			
340.00	a	6815 ± 9	420.00		5961 ± 10	500.00	a	5059 ± 44		
hexadec-1-ene										
298.15	a	9460 ± 748	380.00	a	8408 ± 127	480.00	7199 ± 16	580.00	a	5710 ± 73
300.00	a	9435 ± 722	400.00	a	8166 ± 73	500.00	6940 ± 22	600.00	a	5333 ± 91
320.00	a	9169 ± 491	420.00	a	7927 ± 39	520.00	6665 ± 31			
340.00	a	8908 ± 325	440.00	a	7689 ± 19	540.00	6372 ± 42			
360.00	a	8655 ± 208	460.00	a	7447 ± 13	560.00	a	6054 ± 57		

*Values at this temperature were calculated with extrapolated vapor pressures determined from the fitted Cox coefficients.

TABLE 10. Thermodynamic properties in the ideal-gas state ($R = 8.31451 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ and $p^\circ = 101.325 \text{ kPa}$)

$\frac{T}{\text{K}}$	$\frac{\Delta_f H_m^\circ}{RT}$	$\frac{\Delta_{\text{imp}} H_m^\circ}{RT}$ ^a	$\frac{\Delta_f S_m^\circ}{R}$	$\frac{\Delta_{\text{imp}} S_m^\circ}{R}$ ^b	$\frac{\Delta_f H_m^\circ}{RT}$	$\frac{\Delta_f S_m^\circ}{R}$	$\frac{\Delta_f G_m^\circ}{RT}$
pent-1-ene							
240.00	^c 28.14 ± 0.03	0.02	39.14 ± 0.06	0.02	-8.31 ± 0.21	-38.14 ± 0.06	29.83 ± 0.22
260.00	^c 26.88 ± 0.03	0.05	40.08 ± 0.06	0.04	-8.39 ± 0.20	-38.89 ± 0.06	30.50 ± 0.20
280.00	^v 25.83 ± 0.04	0.09	40.98 ± 0.07	0.06	-8.47 ± 0.18	-39.59 ± 0.07	31.12 ± 0.19
298.15	25.03 ± 0.05	0.14	41.78 ± 0.08	0.10	-8.54 ± 0.17	-40.19 ± 0.08	31.65 ± 0.18
300.00	24.96 ± 0.05	0.14	41.86 ± 0.08	0.10	-8.54 ± 0.17	-40.25 ± 0.08	31.71 ± 0.18
320.00	^d 24.23 ± 0.07	0.22	42.73 ± 0.09	0.16	-8.60 ± 0.17	-40.85 ± 0.09	32.25 ± 0.17
340.00	^{c,d} 23.63 ± 0.09	0.32	43.58 ± 0.11	0.23	-8.64 ± 0.17	-41.41 ± 0.11	32.77 ± 0.17
350.00	^{c,d} 23.37 ± 0.10	0.38	44.00 ± 0.12	0.27	-8.65 ± 0.18	-41.67 ± 0.12	33.02 ± 0.16
cis-pent-2-ene							
240.00	^c 29.20 ± 0.03	0.02	39.09 ± 0.06	0.01	-10.75 ± 0.21	-38.18 ± 0.06	27.44 ± 0.21
260.00	^c 27.80 ± 0.03	0.04	39.97 ± 0.06	0.03	-10.70 ± 0.19	-38.99 ± 0.06	28.29 ± 0.20
280.00	26.64 ± 0.04	0.07	40.83 ± 0.06	0.05	-10.66 ± 0.18	-39.74 ± 0.06	29.09 ± 0.19
298.15	25.75 ± 0.05	0.11	41.59 ± 0.07	0.08	-10.63 ± 0.17	-40.38 ± 0.07	29.75 ± 0.18
300.00	^d 25.67 ± 0.05	0.12	41.67 ± 0.07	0.09	-10.62 ± 0.17	-40.44 ± 0.07	29.82 ± 0.18
320.00	^d 24.86 ± 0.06	0.19	42.49 ± 0.08	0.14	-10.59 ± 0.16	-41.09 ± 0.08	30.50 ± 0.17
340.00	^d 24.18 ± 0.08	0.28	43.31 ± 0.10	0.20	-10.55 ± 0.17	-41.68 ± 0.10	31.13 ± 0.16
350.00	^{c,d} 23.89 ± 0.10	0.33	43.71 ± 0.11	0.24	-10.52 ± 0.17	-41.96 ± 0.11	31.44 ± 0.16
trans-pent-2-ene							
240.00	^c 29.27 ± 0.03	0.02	38.57 ± 0.06	0.01	-13.33 ± 0.23	-38.71 ± 0.06	25.37 ± 0.24
260.00	^c 27.97 ± 0.03	0.04	39.56 ± 0.06	0.03	-12.98 ± 0.22	-39.41 ± 0.06	26.43 ± 0.22
280.00	26.88 ± 0.04	0.07	40.50 ± 0.06	0.05	-12.70 ± 0.20	-40.08 ± 0.06	27.38 ± 0.21
298.15	26.04 ± 0.05	0.11	41.32 ± 0.07	0.08	-12.48 ± 0.19	-40.65 ± 0.07	28.17 ± 0.20
300.00	25.96 ± 0.05	0.12	41.40 ± 0.07	0.09	-12.46 ± 0.19	-40.71 ± 0.07	28.25 ± 0.20
320.00	^d 25.18 ± 0.06	0.19	42.28 ± 0.08	0.13	-12.26 ± 0.18	-41.30 ± 0.08	29.04 ± 0.19
340.00	^d 24.52 ± 0.08	0.28	43.12 ± 0.10	0.20	-12.09 ± 0.18	-41.86 ± 0.10	29.77 ± 0.18
350.00	^{c,d} 24.22 ± 0.10	0.33	43.54 ± 0.11	0.24	-12.01 ± 0.18	-42.13 ± 0.11	30.12 ± 0.18
2-methylbut-1-ene							
240.00	^c 28.66 ± 0.03	0.02	38.11 ± 0.06	0.02	-15.24 ± 0.25	-39.16 ± 0.06	23.92 ± 0.26
260.00	^c 27.41 ± 0.03	0.04	39.11 ± 0.06	0.03	-14.73 ± 0.23	-39.86 ± 0.06	25.12 ± 0.24
280.00	26.37 ± 0.04	0.08	40.06 ± 0.06	0.06	-14.32 ± 0.22	-40.52 ± 0.06	26.20 ± 0.22
298.15	^d 25.55 ± 0.05	0.13	40.87 ± 0.07	0.09	-14.01 ± 0.21	-41.10 ± 0.07	27.09 ± 0.21
300.00	^d 25.48 ± 0.05	0.13	40.96 ± 0.07	0.10	-13.98 ± 0.21	-41.15 ± 0.07	27.17 ± 0.21
320.00	^d 24.72 ± 0.07	0.21	41.82 ± 0.09	0.15	-13.69 ± 0.20	-41.75 ± 0.09	28.06 ± 0.20
340.00	^{c,d} 24.08 ± 0.09	0.31	42.66 ± 0.10	0.22	-13.44 ± 0.20	-42.32 ± 0.10	28.88 ± 0.19
350.00	^{c,d} 23.79 ± 0.10	0.36	43.08 ± 0.11	0.26	-13.33 ± 0.20	-42.59 ± 0.11	29.26 ± 0.19
3-methylbut-1-ene							
240.00	^c 26.70 ± 0.03	0.03	37.64 ± 0.05	0.02	-11.50 ± 0.21	-39.63 ± 0.05	28.13 ± 0.21
260.00	^c 25.57 ± 0.03	0.06	38.60 ± 0.06	0.05	-11.32 ± 0.19	-40.36 ± 0.06	29.04 ± 0.20
280.00	24.64 ± 0.04	0.11	39.53 ± 0.07	0.08	-11.17 ± 0.18	-41.05 ± 0.07	29.88 ± 0.19
298.15	23.93 ± 0.06	0.17	40.35 ± 0.08	0.12	-11.06 ± 0.17	-41.63 ± 0.08	30.57 ± 0.18
300.00	^d 23.86 ± 0.06	0.18	40.43 ± 0.08	0.13	-11.05 ± 0.17	-41.68 ± 0.08	30.64 ± 0.18
320.00	^d 23.22 ± 0.08	0.27	41.31 ± 0.09	0.19	-10.93 ± 0.17	-42.27 ± 0.09	31.34 ± 0.17
340.00	^{c,d} 22.68 ± 0.10	0.38	42.18 ± 0.11	0.27	-10.82 ± 0.18	-42.81 ± 0.11	31.99 ± 0.16
350.00	^{c,d} 22.46 ± 0.12	0.45	42.61 ± 0.13	0.32	-10.76 ± 0.18	-43.06 ± 0.13	32.30 ± 0.16
2-methylbut-2-ene							
240.00	^c 29.24 ± 0.03	0.02	38.15 ± 0.06	0.01	-18.03 ± 0.35	-39.13 ± 0.06	21.10 ± 0.35
260.00	^c 27.87 ± 0.03	0.04	39.06 ± 0.06	0.03	-17.39 ± 0.32	-39.91 ± 0.06	22.52 ± 0.33
280.00	26.72 ± 0.04	0.07	39.94 ± 0.06	0.05	-16.85 ± 0.30	-40.64 ± 0.06	23.78 ± 0.31
298.15	25.85 ± 0.05	0.12	40.71 ± 0.07	0.09	-16.43 ± 0.29	-41.26 ± 0.07	24.83 ± 0.29
300.00	25.76 ± 0.05	0.12	40.79 ± 0.07	0.09	-16.39 ± 0.28	-41.32 ± 0.07	24.93 ± 0.29
320.00	^d 24.96 ± 0.06	0.19	41.63 ± 0.08	0.14	-15.98 ± 0.27	-41.95 ± 0.08	25.97 ± 0.27
340.00	^d 24.29 ± 0.08	0.29	42.45 ± 0.10	0.21	-15.61 ± 0.26	-42.54 ± 0.10	26.92 ± 0.26
350.00	^{c,d} 23.99 ± 0.10	0.34	42.86 ± 0.11	0.25	-15.44 ± 0.26	-42.81 ± 0.11	27.37 ± 0.25

TABLE 10. Thermodynamic properties in the ideal-gas state ($R = 8.31451 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ and $p^\circ = 101.325 \text{ kPa}$) — Continued

$\frac{T}{\text{K}}$	$\frac{\Delta_f^\circ H_m^\circ}{RT}$	$\frac{\Delta_{\text{imp}}^\circ H_m^\circ}{RT}$ ^a	$\frac{\Delta_f^\circ S_m^\circ}{R}$	$\frac{\Delta_{\text{imp}}^\circ S_m^\circ}{R}$ ^b	$\frac{\Delta_f^\circ H_m^\circ}{RT}$	$\frac{\Delta_f^\circ S_m^\circ}{R}$	$\frac{\Delta_f^\circ G_m^\circ}{RT}$
hex-1-ene							
250.00	^c 32.74 ± 0.04	0.01	43.83 ± 0.07	0.01	-16.89 ± 0.35	-49.92 ± 0.07	33.04 ± 0.36
260.00	^c 32.04 ± 0.04	0.02	44.40 ± 0.07	0.02	-16.67 ± 0.34	-50.36 ± 0.07	33.70 ± 0.34
280.00	^c 30.81 ± 0.04	0.04	45.50 ± 0.07	0.03	-16.27 ± 0.31	-51.19 ± 0.07	34.91 ± 0.32
298.15	29.89 ± 0.04	0.07	46.49 ± 0.07	0.05	-15.95 ± 0.30	-51.88 ± 0.07	35.93 ± 0.30
300.00	29.80 ± 0.04	0.07	46.59 ± 0.08	0.05	-15.92 ± 0.29	-51.95 ± 0.08	36.02 ± 0.30
320.00	^d 28.97 ± 0.05	0.12	47.64 ± 0.08	0.09	-15.61 ± 0.28	-52.65 ± 0.08	37.04 ± 0.28
340.00	^{c,d} 28.27 ± 0.06	0.18	48.69 ± 0.09	0.13	-15.32 ± 0.26	-53.30 ± 0.09	37.98 ± 0.27
350.00	^{c,d} 27.97 ± 0.07	0.22	49.20 ± 0.10	0.16	-15.18 ± 0.26	-53.60 ± 0.10	38.42 ± 0.26
cis-hex-2-ene							
250.00	^c 33.86 ± 1.20	0.01	44.51 ± 1.20	0.01	-19.01 ± 1.25	-49.25 ± 1.20	30.24 ± 0.37
260.00	^c 32.96 ± 0.72	0.02	44.91 ± 0.72	0.01	-18.87 ± 0.80	-49.85 ± 0.72	30.98 ± 0.36
280.00	^c 31.39 ± 0.23	0.03	45.74 ± 0.24	0.02	-18.59 ± 0.40	-50.96 ± 0.24	32.37 ± 0.33
298.15	30.22 ± 0.11	0.06	46.50 ± 0.13	0.04	-18.34 ± 0.32	-51.87 ± 0.13	33.53 ± 0.31
300.00	30.11 ± 0.11	0.06	46.58 ± 0.12	0.04	-18.32 ± 0.32	-51.95 ± 0.12	33.64 ± 0.31
320.00	^d 29.07 ± 0.07	0.10	47.44 ± 0.09	0.07	-18.04 ± 0.29	-52.85 ± 0.09	34.81 ± 0.29
340.00	^d 28.22 ± 0.10	0.16	48.34 ± 0.12	0.11	-17.75 ± 0.28	-53.65 ± 0.12	35.90 ± 0.28
350.00	^{c,d} 27.86 ± 0.14	0.19	48.79 ± 0.16	0.14	-17.61 ± 0.29	-54.01 ± 0.16	36.40 ± 0.27
2,3-dimethylbut-2-ene							
250.00	^c 33.20 ± 0.05	0.01	41.21 ± 0.07	0.01	-30.43 ± 0.38	-52.55 ± 0.07	22.12 ± 0.38
260.00	^c 32.48 ± 0.04	0.01	41.78 ± 0.06	0.01	-29.67 ± 0.36	-52.98 ± 0.06	23.30 ± 0.37
280.00	^c 31.23 ± 0.04	0.03	42.89 ± 0.06	0.02	-28.35 ± 0.34	-53.80 ± 0.06	25.45 ± 0.34
298.15	^c 30.25 ± 0.04	0.05	43.85 ± 0.07	0.03	-27.32 ± 0.32	-54.52 ± 0.07	27.20 ± 0.32
300.00	^c 30.16 ± 0.04	0.05	43.94 ± 0.07	0.04	-27.23 ± 0.32	-54.59 ± 0.07	27.37 ± 0.32
320.00	29.25 ± 0.05	0.09	44.94 ± 0.07	0.06	-26.26 ± 0.30	-55.35 ± 0.07	29.09 ± 0.30
340.00	^d 28.46 ± 0.06	0.14	45.91 ± 0.08	0.10	-25.42 ± 0.28	-56.08 ± 0.08	30.65 ± 0.29
360.00	^{c,d} 27.77 ± 0.07	0.21	46.83 ± 0.09	0.15	-24.70 ± 0.27	-56.78 ± 0.09	32.08 ± 0.27
380.00	^{c,d} 27.17 ± 0.09	0.30	47.72 ± 0.11	0.21	-24.05 ± 0.26	-57.44 ± 0.11	33.39 ± 0.26
400.00	^{c,d} 26.66 ± 0.12	0.41	48.60 ± 0.13	0.29	-23.47 ± 0.26	-58.08 ± 0.13	34.61 ± 0.26
hept-1-ene							
250.00	^c 37.91 ± 0.11	0.01	48.00 ± 0.12	0.00	-27.77 ± 0.28	-61.38 ± 0.12	33.62 ± 0.27
260.00	^c 37.10 ± 0.07	0.01	48.67 ± 0.10	0.01	-27.19 ± 0.26	-61.89 ± 0.10	34.69 ± 0.26
280.00	^c 35.71 ± 0.05	0.02	49.98 ± 0.08	0.01	-26.16 ± 0.23	-62.83 ± 0.08	36.67 ± 0.24
298.15	34.67 ± 0.04	0.03	51.14 ± 0.08	0.03	-25.33 ± 0.22	-63.62 ± 0.08	38.29 ± 0.23
300.00	34.57 ± 0.04	0.04	51.26 ± 0.08	0.03	-25.26 ± 0.22	-63.70 ± 0.08	38.44 ± 0.23
320.00	^d 33.63 ± 0.05	0.06	52.52 ± 0.08	0.05	-24.45 ± 0.20	-64.50 ± 0.08	40.05 ± 0.22
340.00	^d 32.85 ± 0.06	0.10	53.76 ± 0.09	0.08	-23.72 ± 0.20	-65.22 ± 0.09	41.51 ± 0.21
350.00	^d 32.52 ± 0.06	0.13	54.37 ± 0.10	0.09	-23.38 ± 0.19	-65.57 ± 0.10	42.19 ± 0.21
oct-1-ene							
260.00	^c 41.98 ± 0.11	0.00	53.04 ± 0.13	0.00	-35.53 ± 0.33	-73.30 ± 0.13	37.77 ± 0.33
280.00	^c 40.42 ± 0.06	0.01	54.53 ± 0.09	0.01	-34.04 ± 0.30	-74.39 ± 0.09	40.35 ± 0.31
298.15	^c 39.25 ± 0.05	0.02	55.87 ± 0.09	0.01	-32.84 ± 0.28	-75.29 ± 0.09	42.45 ± 0.29
300.00	^c 39.15 ± 0.05	0.02	56.00 ± 0.09	0.01	-32.72 ± 0.28	-75.38 ± 0.09	42.65 ± 0.29
320.00	^d 38.10 ± 0.05	0.03	57.44 ± 0.09	0.03	-31.55 ± 0.26	-76.28 ± 0.09	44.73 ± 0.27
340.00	^d 37.24 ± 0.05	0.06	58.87 ± 0.10	0.04	-30.50 ± 0.24	-77.11 ± 0.10	46.61 ± 0.26
360.00	^d 36.54 ± 0.07	0.10	60.28 ± 0.11	0.07	-29.54 ± 0.24	-77.86 ± 0.11	48.32 ± 0.25
non-1-ene							
298.15	^c 44.39 ± 0.07	0.01	60.51 ± 0.11	0.01			
300.00	^c 44.27 ± 0.07	0.01	60.66 ± 0.10	0.01			
320.00	^c 43.07 ± 0.06	0.02	62.28 ± 0.10	0.01			
340.00	42.10 ± 0.06	0.03	63.89 ± 0.10	0.03			
360.00	41.30 ± 0.06	0.06	65.47 ± 0.11	0.04			
380.00	40.64 ± 0.07	0.09	67.03 ± 0.12	0.07			
400.00	^d 40.11 ± 0.07	0.14	68.57 ± 0.12	0.11			
420.00	^d 39.68 ± 0.09	0.21	70.09 ± 0.13	0.16			
440.00	^{c,d} 39.33 ± 0.11	0.30	71.59 ± 0.15	0.22			
450.00	^{c,d} 39.19 ± 0.12	0.35	72.33 ± 0.16	0.26			

TABLE 10. Thermodynamic properties in the ideal-gas state ($R = 8.31451 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ and $p^\circ = 101.325 \text{ kPa}$) — Continued

T K	$\frac{\Delta_f H_m^\circ}{R T}$	$\frac{\Delta_{\text{imp}} H_m^\circ}{R T}$ ^a	$\frac{\Delta_f S_m^\circ}{R}$	$\frac{\Delta_{\text{imp}} S_m^\circ}{R}$ ^b	$\frac{\Delta_f H_m^\circ}{R T}$	$\frac{\Delta_f S_m^\circ}{R}$	$\frac{\Delta_f G_m^\circ}{R T}$	
dec-1-ene								
298.15	c,e	49.09 ± 0.10	0.00	65.35 ± 0.13	0.00	-49.77 ± 0.42	-98.59 ± 0.13	48.82 ± 0.42
298.15	c	48.91 ± 0.22	0.00	65.18 ± 0.23	0.00	-49.95 ± 0.46	-98.77 ± 0.23	48.82 ± 0.42
300.00	c	48.78 ± 0.20	0.00	65.35 ± 0.22	0.00	-49.74 ± 0.45	-98.87 ± 0.22	49.13 ± 0.42
320.00	c	47.49 ± 0.11	0.01	67.16 ± 0.14	0.01	-47.73 ± 0.39	-100.00 ± 0.14	52.28 ± 0.40
340.00	c	46.43 ± 0.07	0.02	68.94 ± 0.12	0.01	-45.92 ± 0.36	-101.03 ± 0.12	55.11 ± 0.38
360.00	d	45.56 ± 0.06	0.04	70.71 ± 0.12	0.03	-44.28 ± 0.34	-101.97 ± 0.12	57.69 ± 0.36
380.00	d	44.87 ± 0.07	0.06	72.46 ± 0.12	0.05	-42.78 ± 0.32	-102.82 ± 0.12	60.04 ± 0.34
400.00	d	44.31 ± 0.08	0.10	74.19 ± 0.13	0.07	-41.40 ± 0.31	-103.60 ± 0.13	62.20 ± 0.33
420.00	d	43.87 ± 0.10	0.15	75.90 ± 0.15	0.11	-40.12 ± 0.30	-104.31 ± 0.15	64.19 ± 0.33
440.00	d	43.54 ± 0.12	0.21	77.61 ± 0.16	0.16	-38.93 ± 0.30	-104.95 ± 0.16	66.02 ± 0.33
450.00	c,d	43.41 ± 0.13	0.26	78.46 ± 0.17	0.19	-38.36 ± 0.30	-105.24 ± 0.17	66.89 ± 0.33
undec-1-ene								
298.15	c	54.19 ± 0.07	0.00	70.02 ± 0.12	0.00			
300.00	c	54.03 ± 0.07	0.00	70.20 ± 0.12	0.00			
320.00	c,d	52.53 ± 0.07	0.00	72.13 ± 0.12	0.00			
340.00	c,d	51.30 ± 0.07	0.01	74.05 ± 0.12	0.01			
350.00	c,d	50.78 ± 0.07	0.01	75.01 ± 0.12	0.01			
dodec-1-ene ^f								
298.15	c,e	58.32 ± 0.11	0.00	75.09 ± 0.14	0.00	-66.72 ± 0.33	-121.65 ± 0.14	54.93 ± 0.35
298.15	c	58.29 ± 0.12	0.00	75.05 ± 0.15	0.00	-66.75 ± 0.34	-121.68 ± 0.15	54.93 ± 0.35
300.00	c	58.12 ± 0.11	0.00	75.24 ± 0.15	0.00	-66.48 ± 0.34	-121.82 ± 0.15	55.34 ± 0.34
320.00	c,d	56.52 ± 0.08	0.00	77.34 ± 0.13	0.00	-63.71 ± 0.31	-123.25 ± 0.13	59.54 ± 0.33
340.00	c,d	55.21 ± 0.08	0.01	79.41 ± 0.13	0.00	-61.22 ± 0.29	-124.55 ± 0.13	63.33 ± 0.31
360.00	c,d	54.16 ± 0.09	0.01	81.49 ± 0.14	0.01	-58.96 ± 0.28	-125.72 ± 0.14	66.76 ± 0.31
380.00	c,d	53.35 ± 0.10	0.02	83.58 ± 0.15	0.02	-56.86 ± 0.27	-126.75 ± 0.15	69.89 ± 0.31
400.00	d	52.72 ± 0.12	0.04	85.68 ± 0.17	0.03	-54.91 ± 0.27	-127.67 ± 0.17	72.76 ± 0.32
hexadec-1-ene ^f								
298.15	c,e	77.86 ± 0.12	0.00	94.04 ± 0.18	0.00	-100.68 ± 0.47	-168.27 ± 0.18	67.59 ± 0.49
360.00	c	72.21 ± 0.59	0.00	102.43 ± 0.60	0.00	-88.41 ± 0.69	-173.85 ± 0.60	85.44 ± 0.42
380.00	c	71.18 ± 0.35	0.00	105.28 ± 0.38	0.00	-85.03 ± 0.49	-175.16 ± 0.38	90.13 ± 0.40
400.00	c,d	70.38 ± 0.21	0.01	108.11 ± 0.26	0.01	-81.93 ± 0.39	-176.34 ± 0.26	94.41 ± 0.39
420.00	c,d	69.79 ± 0.14	0.02	110.94 ± 0.21	0.01	-79.06 ± 0.35	-177.40 ± 0.21	98.34 ± 0.38
440.00	c,d	69.37 ± 0.13	0.03	113.75 ± 0.21	0.02	-76.38 ± 0.33	-178.34 ± 0.21	101.95 ± 0.39
460.00	d	69.11 ± 0.15	0.05	116.57 ± 0.23	0.04	-73.87 ± 0.32	-179.16 ± 0.23	105.29 ± 0.39
480.00	d	68.98 ± 0.17	0.08	119.39 ± 0.25	0.06	-71.48 ± 0.33	-179.87 ± 0.25	108.38 ± 0.41
500.00	d	68.99 ± 0.20	0.12	122.21 ± 0.27	0.09	-69.22 ± 0.33	-180.48 ± 0.27	111.25 ± 0.42

^aGas-imperfection correction included in the ideal-gas enthalpy.^bGas-imperfection correction included in the ideal-gas entropy.^cValues at this temperature were calculated with extrapolated vapor pressures calculated from the fitted Cox coefficients.^dValues at this temperature were calculated with graphically extrapolated values of the liquid-phase heat capacities.^eValues at this temperature were calculated with the measured enthalpy-of-vaporization value listed in Table 5.^fValues of the entropy for the liquid phase employed in these calculations were increased by $R \cdot \ln 2 = 0.693$ to "correct" for the effect of disorder in the crystals during condensed-phase heat-capacity studies. See Sec. 5.2.

TABLE 11. Comparison of enthalpies of isomerization $\Delta_{\text{isom}}H_m^\circ$ at 298.15 K.^{a,b,c,d}

Reactant/Product		Source/ $\Delta_{\text{isom}}H_m^\circ$ at 298.15 K			
pent-1-ene to:	Table 7			84WIB/WAS	
<i>cis</i> -pent-2-ene	-6.5 ± 0.8			-6.4 ± 0.1	
<i>trans</i> -pent-2-ene	-11.0 ± 0.9			-11.3 ± 0.1	
2-methylbut-1-ene to:	Table 7			91WIB/HAO	
2-methylbut-2-ene	-7.1 ± 1.7			-7.6 ± 0.3	
hex-1-ene to:	Table 7	87ROG/CRO	83ROG/CRO	81WIB/WAS	75ROG/PAP
<i>cis</i> -hex-2-ene	-7.5 ± 1.9 ^e	-7.2 ± 0.9	-7.6 ± 1.1	-7.8 ± 0.4	-10.1 ± 1.2
<i>trans</i> -hex-2-ene	-13.1 ± 2.0	-10.6 ± 0.7	-11.6 ± 1.2	-10.9 ± 0.4	-12.1 ± 1.4
<i>cis</i> -hex-3-ene	-6.6 ± 1.8	-5.1 ± 0.9	-5.5 ± 1.2	-5.7 ± 0.4	-4.0 ± 1.5
<i>trans</i> -hex-3-ene	-13.7 ± 1.8	-8.8 ± 0.9	-8.7 ± 1.1	-9.8 ± 0.3	-13.5 ± 1.9
2-methylpent-1-ene to:	Table 7	87ROG/CRO			
4-methylpent-1-ene	9.9 ± 2.2	10.4 ± 0.6			
2-methylpent-2-ene	-8.6 ± 1.9	-4.7 ± 0.9			
4-methyl- <i>cis</i> -pent-2-ene	2.9 ± 1.7	0.6 ± 0.6			
4-methyl- <i>trans</i> -pent-2-ene	-1.6 ± 1.8	-2.1 ± 0.7			
3-methylpent-1-ene to:	Table 7	87ROG/CRO			
4-methyl- <i>cis</i> -pent-2-ene	-16.2 ± 1.9	-14.0 ± 0.7			
4-methyl- <i>trans</i> -pent-2-ene	-16.6 ± 2.0	-14.5 ± 0.8			
2,3-dimethylbut-1-ene to:	Table 7	87ROG/CRO		91WIB/HAO	
2,3-dimethylbut-2-ene	-6.8 ± 1.1	-7.6 ± 0.6		-7.8 ± 0.2	
hept-1-ene to:	Table 7	88ROG/DEJ		84WIB/WAS	
<i>cis</i> -hept-2-ene	-6.8 ± 1.1	-7.3 ± 0.6		-8.3 ± 0.1	
<i>trans</i> -hept-2-ene	-11.2 ± 1.1	-11.1 ± 0.7		-11.7 ± 0.1	
<i>cis</i> -hept-3-ene	5.9 ± 1.0	6.7 ± 0.6		-6.8 ± 0.1	
<i>trans</i> -hept-3-ene	-11.0 ± 1.2	-10.5 ± 0.6		-10.8 ± 0.1	

^aAll values are in kJ·mol⁻¹.

^bValues for the enthalpy of isomerization are listed relative to the first compound given in each subsection.

^cUncertainties are twice the standard deviation of the mean and for the combustion calorimetry (column 2) are derived from the uncertainty intervals listed for the enthalpies of combustion in Table 7.

^dColumn 2 is derived from combustion calorimetric measurements, columns 3 and 4 from hydrogen reaction calorimetric measurements, and column 5 from hydration reaction calorimetry.

^eThis value was calculated with the "revised" enthalpy of combustion listed in Table 7. The corresponding value would be (-11.5 ± 1.9)kJ·mol⁻¹, if the combustion results of 56BAR were used in the calculations.

TABLE 12. Comparison of ideal-gas $\Delta_f H_m^\circ$ values at 298.15 K derived from measurements and group-additivity^a

Compound	$\Delta_f H_m^\circ$ (kJ·mol ⁻¹)	Σ groups	$\Delta_f H_m^\circ - \Sigma$ groups
PENTENES			
pent-1-ene	-21.17 ± 0.87	-20.68	-0.49
<i>cis</i> -pent-2-ene	-26.35 ± 0.83	-25.91	-0.44
<i>trans</i> -pent-2-ene	-30.94 ± 0.94	-32.41	1.47
2-methylbut-1-ene	-34.73 ± 1.02	-34.83	0.10
3-methylbut-1-ene	-27.42 ± 0.85	-28.43	1.01
2-methylbut-2-ene	-40.73 ± 1.41	-40.85	0.12
HEXENES			
hex-1-ene	-39.54 ± 1.46	-41.40	1.86
<i>cis</i> -hex-2-ene	-45.5 ± 1.6	-46.63	1.1 ^b
<i>trans</i> -hex-2-ene	-51.71 ± 1.69	-53.13	1.42
<i>cis</i> -hex-3-ene	-45.51 ± 1.46	-45.84	0.33
<i>trans</i> -hex-3-ene	-52.30 ± 1.46	-52.34	0.04
2-methylpent-1-ene	-57.24 ± 1.43	-55.55	-1.69
3-methylpent-1-ene	-47.26 ± 1.66	-49.15	1.89
4-methylpent-1-ene	-49.06 ± 1.88	-50.11	1.05
2-methylpent-2-ene	-64.72 ± 1.58	-60.78	-3.94
3-methyl- <i>cis</i> -pent-2-ene	-60.07 ± 1.61	-60.78	0.71
3-methyl- <i>trans</i> -pent-2-ene	-60.95 ± 1.39	-60.78	-0.17
4-methyl- <i>cis</i> -pent-2-ene	-55.28 ± 1.35	-54.38	-0.90
4-methyl- <i>trans</i> -pent-2-ene	-59.32 ± 1.50	-60.88	1.56
2-ethylbut-1-ene	-53.72 ± 1.61	-54.76	1.04
2,3-dimethylbut-1-ene	-64.16 ± 1.81	-63.30	-0.86
3,3-dimethylbut-1-ene	-59.38 ± 1.66	-57.40	-1.98
2,3-dimethylbut-2-ene	-67.73 ± 1.58	-69.22	1.49
HEPTENES			
hept-1-ene	-62.81 ± 1.08	-62.12	-0.69
<i>cis</i> -hept-2-ene	-68.83 ± 1.08	-67.35	-1.48
<i>trans</i> -hept-2-ene	-73.21 ± 1.04	-73.85	0.64
<i>cis</i> -hept-3-ene	-68.43 ± 0.99	-66.56	-1.87
<i>trans</i> -hept-3-ene	-73.42 ± 1.17	-73.06	-0.36
2,4-dimethylpent-2-ene	-88.84 ± 1.11	-89.25	0.41
3-methyl- <i>cis</i> -hex-3-ene	-79.61 ± 1.15	-80.71	1.10
3-methyl- <i>trans</i> -hex-3-ene	-77.01 ± 1.11	-80.71	3.70
4,4-dimethylpent-1-ene	-79.35 ± 1.83	-82.27	2.92
2,4-dimethylpent-1-ene	-83.89 ± 1.37	-84.98	1.09
4,4-dimethyl- <i>cis</i> -pent-2-ene	-72.66 ± 1.41	-70.85	-1.81
4,4-dimethyl- <i>trans</i> -pent-2-ene	-88.86 ± 1.11	-89.85	0.99
3-methyl-2-ethylbut-1-ene	-79.65 ± 1.54	-83.23	3.58
2,3,3-trimethylbut-1-ene	-85.52 ± 1.37	-92.27	6.75
OCTENES			
oct-1-ene	-81.41 ± 1.37	-82.84	1.43
2-methyl-3-ethylpent-1-ene	-100.41 ± 1.08	-104.74	4.33
2,2-dimethyl- <i>cis</i> -hex-3-ene	-89.50 ± 2.51	-90.78	1.28
2,2-dimethyl- <i>trans</i> -hex-3-ene	-107.90 ± 1.49	-109.78	1.88
2,4,4-trimethylpent-1-ene	-110.00 ± 1.04	-110.74	0.74
2,4,4-trimethylpent-2-ene	-105.12 ± 1.92	-105.72	0.60
HIGHER ALKENES			
dec-1-ene	-123.38 ± 2.03	-124.28	0.90
2,2,5,5-tetramethyl- <i>trans</i> -hex-3-ene	-165.64 ± 4.00	-167.22	1.58
dodec-1-ene	-165.40 ± 1.61	-165.72	0.32
hexadec-1-ene	-249.59 ± 2.28	-248.60	-0.99

^aGas-imperfection corrections required to derive the ideal-gas enthalpies of formation are significant at 298.15 K for all alkenes smaller than C₁₀. The magnitudes of the gas-imperfection corrections may be seen by comparing the gas-phase values listed in Table 7 with the ideal-gas values listed here.

^bThe difference is -2.9 kJ·mol⁻¹ if calculated with the enthalpy of combustion reported by Bartolo (56BAR) rather than the revised value listed in Table 7.

TABLE 13. Comparison of ideal-gas entropy S_m° values at 298.15 K derived from measurements and group-additivity

Compound	S_m°/R	$[S_m^\circ(\text{alkene}) - \Sigma \text{ groups}]/R$	$[S_m^\circ(\text{alkane}) - \Sigma \text{ groups}]/R^a$
pent-1-ene	41.78 ± 0.08	-0.03	-0.01
cis-pent-2-ene	41.59 ± 0.07	-0.26	
trans-pent-2-ene	41.32 ± 0.07	-0.07	
2-methylbut-1-ene	40.87 ± 0.07	0.00	
3-methylbut-1-ene	40.35 ± 0.08	-0.10	
2-methylbut-2-ene	40.71 ± 0.07	-0.01	
hex-1-ene	46.49 ± 0.07	-0.06	0.02
cis-hex-2-ene	46.58 ± 0.12	-0.01	
2,3-dimethylbut-2-ene	43.85 ± 0.07	0.25	
hept-1-ene	51.14 ± 0.08	-0.16	0.01
oct-1-ene	55.87 ± 0.09	-0.17	-0.02
non-1-ene	60.51 ± 0.11	-0.27	-0.03
dec-1-ene	65.35 ± 0.13 b	-0.18	-0.05
undec-1-ene	70.02 ± 0.12	-0.25 c	
dodec-1-ene	74.39 ± 0.16 b	0.07 (-0.62) d	0.03
hexadec-1-ene	93.35 ± 0.18 b	0.05 (-0.64) d	-0.03

^aIdeal-gas entropies at 298.15 K for the normal alkanes based on calorimetric data were derived as described in Appendix 2. All data sources are provided there.

^bThis value was calculated with the measured enthalpy of vaporization value listed in Table 5. All other values listed in this column were calculated with enthalpies of vaporization calculated from measured vapor pressures and the Cox and Clapeyron equations. See Sec. 2.2.b.

^cAn ideal-gas entropy based on calorimetric data could not be derived for undecane because of the poor quality of the available vapor pressures. See Appendix 2.

^dThe value in brackets is obtained, if the experimental values are not "corrected" for disorder in the crystals during the condensed-phase heat-capacity studies. See Sec. 5.2.

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Appendix 1. Vapor-Pressure Data Not Used in Cox-Equation Fits

Vapor-pressure data not used in the Cox-equation fits for the alkenes are compared with the fitted equations in Figs. 12 through 25. The bold, black arrows indicate the temperature range of the vapor pressures used in the fits. Clearly, long extrapolations (sometimes in excess of 100 K) were involved in the comparisons for several of the data sets. When such long extrapolations are involved, the comparisons show only that the data sets are inconsistent. The short temperature range of many of the fitted vapor pressure data sets (see Table 2) makes such long extrapolations extremely tenuous.

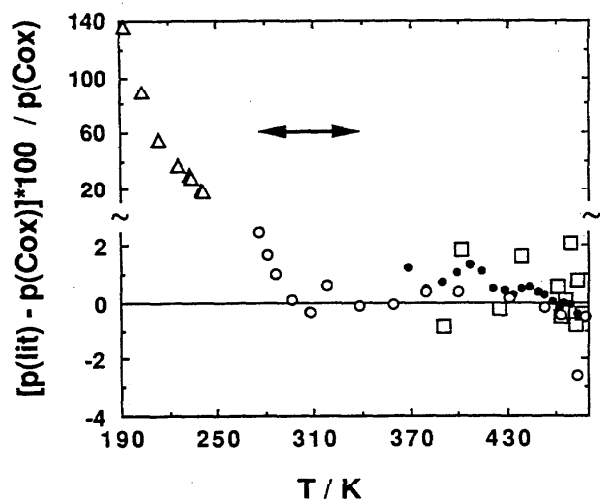


FIG. 12. Deviations of literature vapor pressures from values calculated with the Cox parameters listed in Table 2 for pent-1-ene. \square , 91PEI/YOU; \bullet , 83WOL/KAY; \circ , 48DAY/NIC; Δ , 41BEN. The double-headed arrow in this and Figs. 12 through 25 indicates the range of the fitted vapor pressures.

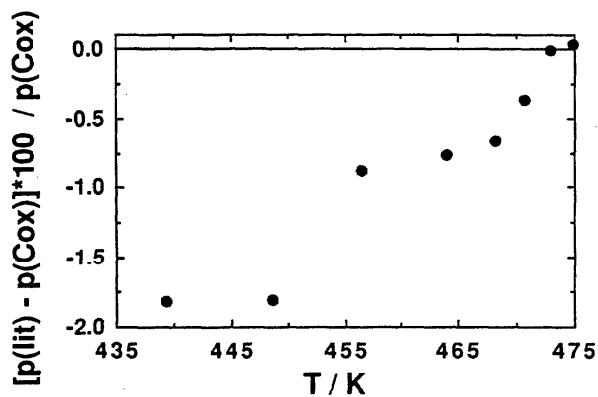


FIG. 13. Deviations of literature vapor pressures from values calculated with the Cox parameters listed in Table 2 for *cis*-pent-2-ene. \bullet , 71LEN/REB. The temperature range of these vapor pressures does not overlap with that of those used in the Cox-equation fit.

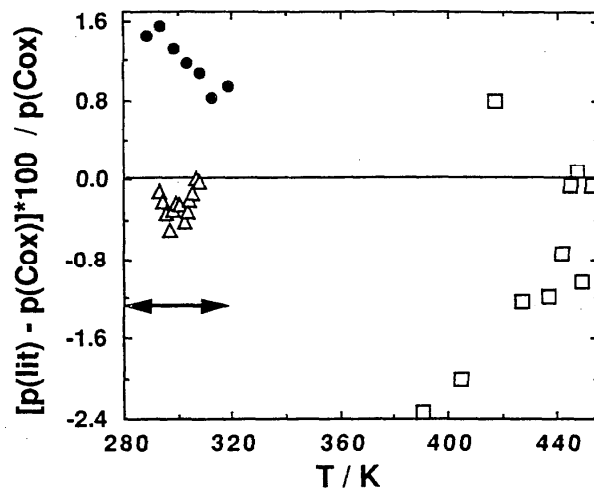


FIG. 14. Deviations of literature vapor pressures from values calculated with the Cox parameters listed in Table 2 for 3-methylbut-1-ene. \square , 91PEI/YOU; \bullet , 68BRA/ODO; Δ , 60GO/KOG.

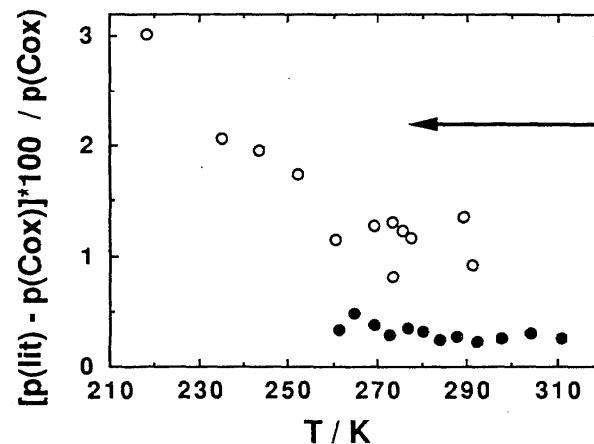


FIG. 15. Deviations of literature vapor pressures from values calculated with the Cox parameters listed in Table 2 for 2-methylbut-2-ene. \bullet , 73BOU; \circ , 40LAM/ROP. One vapor pressure value at 194 K from 40LAM/ROP is not shown; it is 8 percent larger than the value derived from the fit.

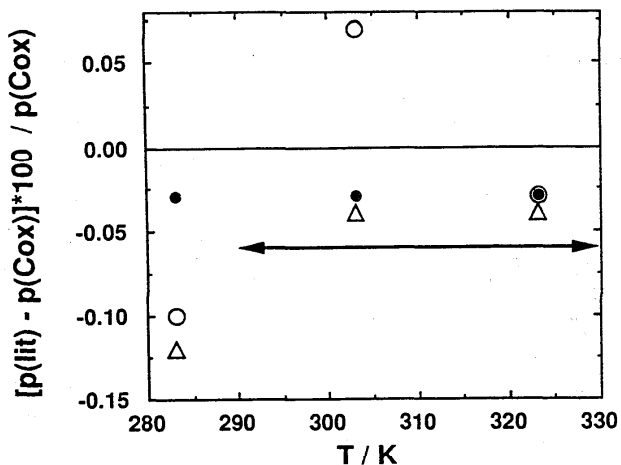


FIG. 16. Deviations of literature vapor pressures measured by Vera and Prausnitz (71VER/PRA) from values calculated with the Cox parameters listed in Table 2. \circ , hex-1-ene; Δ , 2-methylpent-1-ene; \bullet , 4-methylpent-1-ene.

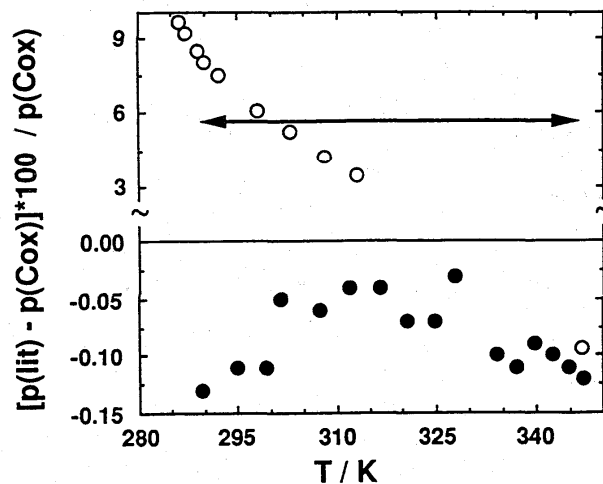


FIG. 18. Deviations of literature vapor pressures from values calculated with the Cox parameters listed in Table 2 for 2,3-dimethylbut-2-ene. \circ , 55CUM/MCD; \bullet , 71BAG/MAL.

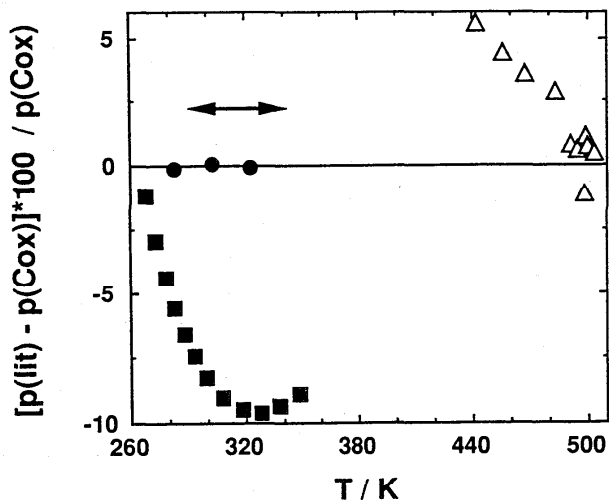


FIG. 17. Deviations of literature vapor pressures from values calculated with the Cox parameters listed in Table 2 for hex-1-ene. Δ 91PEI/YOU; \bullet , 71VER/PRA; \blacksquare , 37MAE/MUF (calculated from equation only). See also Fig16.

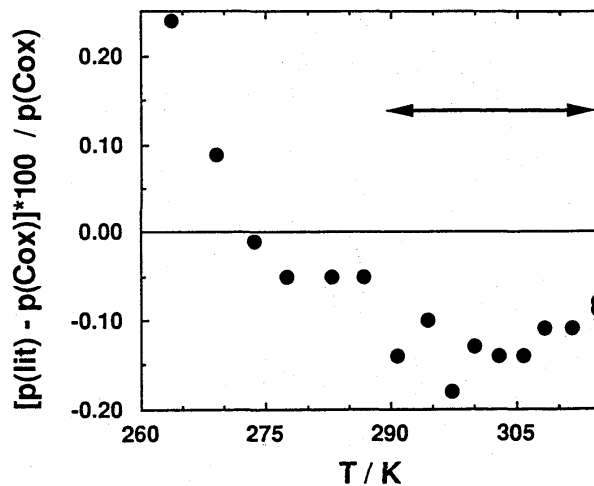


FIG. 19. Deviations of literature vapor pressures from values calculated with the Cox parameters listed in Table 2 for 3,3-dimethylbut-1-ene. \bullet , 71BAG/MAL.

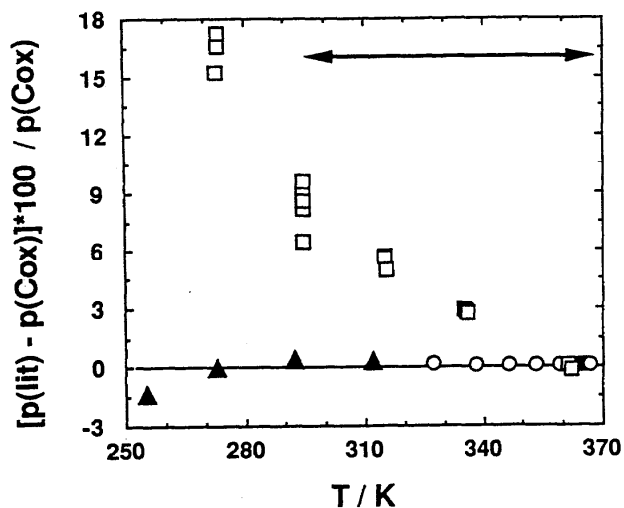


FIG. 20. Deviations of literature vapor pressures from values calculated with the Cox parameters listed in Table 2 for hept-1-ene. \circ , 70EIS/ORO; \blacktriangle , 41LIS; \square , 36BEN/CUT. See FIG. 21, also.

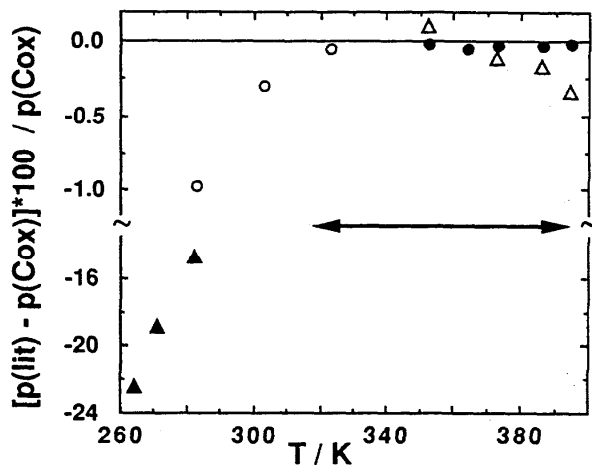


FIG. 22. Deviations of literature vapor pressures from values calculated with the Cox parameters listed in Table 2 for oct-1-ene. \circ , 71VER/PRA; \bullet , 74MIC/ELW; \triangle , 78MIH/KIR; \blacktriangle , 31LIN.

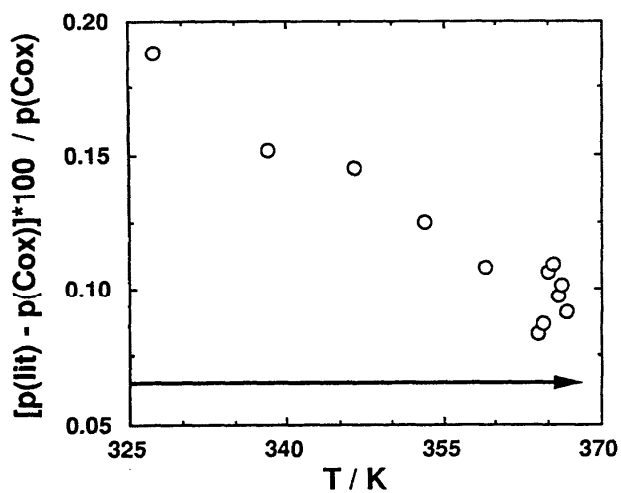


FIG. 21. Deviations of vapor pressures from reference 70EIS/ORO from values calculated with the Cox parameters listed in Table 2 for hept-1-ene. \circ , 70EIS/ORO. See FIG. 20, also.

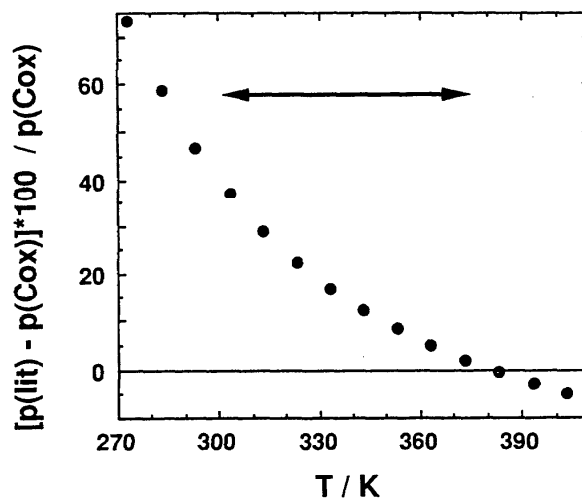


FIG. 23. Deviations of literature vapor pressures from values calculated with the Cox parameters listed in Table 2 for 2,4,4-trimethylpent-1-ene. \bullet , 52YOR/FEL.

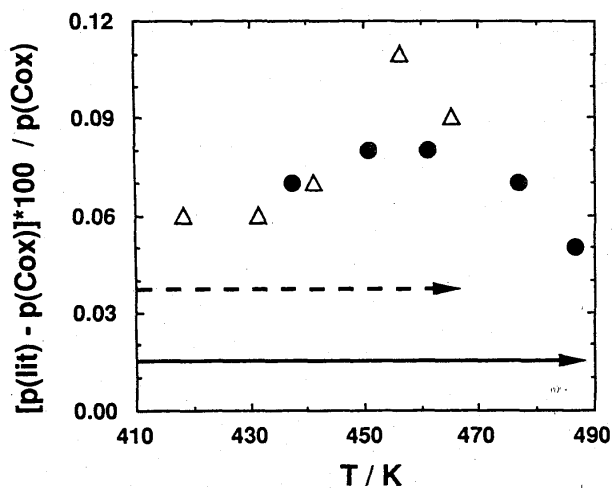


FIG. 24. Deviations of literature vapor pressures from values calculated with the Cox parameters listed in Table 2 for undec-1-ene and dodec-1-ene. Δ , undec-1-ene (83ELV/KUU); \bullet , dodec-1-ene (83ELV/KUU). The dashed arrow indicates the range of the data used in the Cox-equation fit for undec-1-ene. The uninterrupted arrow is the range for dodec-1-ene.

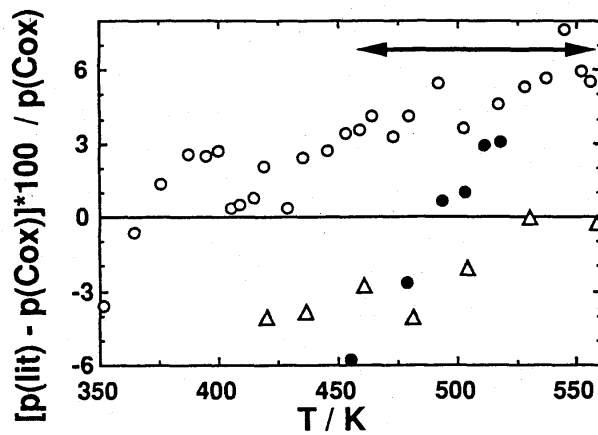


FIG. 25. Deviations of literature vapor pressures from values calculated with the Cox parameters listed in Table 2 for hexadec-1-ene. \circ , 55MYE/FEN; \bullet , 54WAR/VAN; Δ , 52KEI/VAN.

Appendix 2. Data Sources for Normal Alkane Entropies

An exhaustive literature search for thermodynamic information for the alkanes was outside the scope of this research. This section briefly describes the origins of the normal-alkane entropy values used to derive results used in Table 13 and Fig. 10.

Entropies at 298.15 K for the liquid phase of the normal alkanes from C₅ to C₁₈ were determined by adiabatic calorimetry by the Thermodynamics Group (at the then Bureau of Mines) in Bartlesville, OK. Values are listed in reference 67MES/GUI, which includes original data for pentane, heptadecane, and octadecane; and updated calculations of thermodynamic functions for the normal alkanes from C₆ to C₁₆. The original sources for the C₆ to C₁₆ compounds are: C₆, 46DOU/HUF; C₇, 61HUF/GRO; and C₈ to C₁₆, 54FIN/GRO.

For the calculation of ideal-gas entropies at 298.15 K for the normal alkanes, entropies of vaporization and vapor pressures (needed for the entropy of compression calculation) are required. Entropies of vaporization for C₅ to C₁₀ were those selected in the critical review by Ma-

jer and Svoboda (85MAJ/SVO). The values listed in 85MAJ/SVO are in excellent accord (within 0.05·R) with values derived from Cox-equation fits of vapor pressures measured by Rossini and co-workers (C₅, C₆, C₈, and C₁₀ from 45WIL/TAY, C₇ and C₉ from 49FOR/NOR). The fitting procedure was the same as that described in Sec. 2.2.b. The critical temperatures and pressures for the normal alkanes listed by Ambrose and Walton (89AMB/WAL) were used, as were critical densities listed in reference 90ANS/GUD. Vapor pressures at 298.15 K were calculated from the fits.

Entropies of vaporization at 298.15 K for C₁₂ and C₁₆ were derived from Cox-equation fits of vapor pressures [C₁₂, (89MOR/KOB, 86ALL/JOS, 45WIL/TAY); C₁₆, (89MOR/KOB, 54CAM/FOR)]. Entropies of compression were calculated with vapor pressures calculated with the fitted parameters. The available vapor pressures for normal undecane are not consistent with those of the other alkanes. This is apparent when the Wagner-equation coefficients listed by Morgan and Kobayashi (89MOR/KOB) are compared with those for the other normal alkanes. No gas-phase values were calculated for undecane.

Appendix 3. Chemical Abstracts Registry Numbers**PENTENES**

pent-1-ene [109-67-1]
trans-pent-2-ene [646-04-8]
3-methylbut-1-ene [563-45-1]
cis-pent-2-ene [627-20-3]
2-methylbut-1-ene [563-46-2]
2-methylbut-2-ene [513-35-9]

HEXENES

hex-1-ene [592-41-6]
trans-hex-2-ene [4050-45-7]
trans-hex-3-ene [13269-52-8]
3-methylpent-1-ene [760-20-3]
2-methylpent-2-ene [625-27-4]
3-methyl-*trans*-pent-2-ene [616-12-6]
4-methyl-*trans*-pent-2-ene [674-76-0]
2,3-dimethylbut-1-ene [563-78-0]
2,3-dimethylbut-2-ene [563-79-1]
cis-hex-2-ene [7688-21-3]
cis-hex-3-ene [7642-09-3]
2-methylpent-1-ene [763-29-1]
4-methylpent-1-ene [691-37-2]
3-methyl-*cis*-pent-2-ene [922-62-3]
4-methyl-*cis*-pent-2-ene [691-38-3]
2-ethylbut-1-ene [760-21-4]
3,3-dimethylbut-1-ene [558-37-2]

HEPTENES

hept-1-ene [592-76-7]
trans-hept-2-ene [14686-13-6]
trans-hept-3-ene [14686-14-7]
2,4-dimethylpent-2-ene [625-65-0]
3-methyl-*trans*-hex-3-ene [3899-36-3]
2,4-dimethylpent-1-ene [2213-32-3]
4,4-dimethyl-*trans*-pent-2-ene [690-08-4]

2,3,3-trimethylbut-1-ene [594-56-9]
cis-hept-2-ene [6443-92-1]
cis-hept-3-ene [7642-10-6]
5-methylhex-1-ene [3524-73-0]
3-methyl-*cis*-hex-3-ene [4914-89-0]
4,4-dimethylpent-1-ene [762-62-9]
4,4-dimethyl-*cis*-pent-2-ene [762-63-0]
3-methyl-2-ethylbut-1-ene [7357-93-9]

OCTENES

oct-1-ene [111-66-0]
2,2-dimethyl-*cis*-hex-3-ene [690-92-6]
2,4,4-trimethylpent-1-ene [107-39-1]
2,5-dimethyl-*cis*-hex-3-ene [10557-44-5]
2-methyl-3-ethylpent-1-ene [19780-66-6]
2,2-dimethyl-*trans*-hex-3-ene [690-93-7]
2,4,4-trimethylpent-2-ene [107-40-4]
2,5-dimethyl-*trans*-hex-3-ene [692-70-6]

NONENES

non-1-ene [124-11-8]

DECENES

dec-1-ene [872-05-9]
2,2,5,5-tetramethyl-*cis*-hex-3-ene [692-47-7]
2,2,5,5-tetramethyl-*trans*-hex-3-ene [692-48-8]

HIGHER ALK-1-ENES

undec-1-ene [821-95-4]
dodec-1-ene [112-41-4]
tridec-1-ene [2437-56-1]
tetradec-1-ene [1120-36-1]
pentadec-1-ene [13360-61-7]
hexadec-1-ene [629-73-2]

ALKANES

undecane [1120-21-4]