HANDBOOK

OF

VAPOR PRESSURES AND HEATS OF VAPORIZATION OF HYDROCARBONS AND RELATED COMPOUNDS

Randolph C. Wilhoit, Ph. D. Bruno J. Zwolinski, Ph. D.

HANDBOOK

OF

VAPOR PRESSURES AND HEATS OF VAPORIZATION

OF

HYDROCARBONS AND RELATED COMPOUNDS

Randolph C. Wilhoit, Ph. D.

Associate Professor of Chemistry, Texas A&M University

Associate Director, Thermodynamics Research Center

Assistant Director, American Petroleum Institute Research Project 44

Bruno J. Zwolinski, Ph. D.

Professor of Chemistry, Texas A&M University
Director, Thermodynamics Research Center

Director, American Petroleum Institute Research Project 44

in collaboration with

George K. Estok, Ph. D. Gisela B. Mahoney, Ph. D. Sharon M. Dregne, B. Sc.

all of

Thermodynamics Research Center Department of Chemistry Texas A&M University College Station, Texas

THERMODYNAMICS RESEARCH CENTER
Department of Chemistry
Texas A&M University
College Station, Texas 77843

1971

Copyright © by the THERMODYNAMICS RESEARCH CENTER and the AMERICAN PETROLEUM INSTITUTE, 1971.

All rights reserved. No part of this publication may be reproduced, stored in a retrieval system, or transmitted in any form or by any means, mechanical, photocopying, electronic or otherwise without prior written permission of the publisher.

Library of Congress Catalog Card Number: 79-169180

Distributed by

Thermodynamics Research Center Data Distribution Office Faculty Exchange Box 130 College Station, Texas 77843

Photo-offset composition by

Annie Lin Risinger, Technical Editor Thermodynamics Research Center Editorial Office

> Printed in the United State of America By Evans Press, Fort Worth, Texas

DEDICATION

To the chairmen and the members of the API Advisory Committee and to the staff members of the

API Research Project 6
National Bureau of Standards and Carnegie-Mellon University

API Research Project 45 The Ohio State University

API Research Projects 48 and 52 U. S. Bureau of Mines Bartlesville Petroleum Research Center Thermodynamics Laboratory

API Research Project 58
Carnegie-Mellon University and The Ohio State University

whose cooperative efforts in the period 1926 through 1966 produced the finest collection of high quality data on physical properties of hydrocarbons and related compounds.

The 1970-71 Advisory Committee Membership

for the

AMERICAN PETROLEUM INSTITUTE RESEARCH PROJECT 44

R. M. Blunden, BP North America, Inc.

D. L. Camin, Sun Oil Company

R. A. Findlay, Phillips Petroleum Company

S. A. Francis, Texaco Incorporated

S. T. Hadden, Monsanto Company, Hydrocarbons Division (retired)

A. C. Jones, Shell Development Company

J. G. Larson, Gulf Research and Development Company

A. S. Trube, Getty Oil Company

J. C. Winfrey, Signal Oil Company

J. P. McCullough, Assistant Chairman, Mobil Research and Development Corporation

W. O. Taff, Chairman, Esso Research and Engineering Company

Committee on API44-TRC Publications in Science and Engineering

S. A. Francis, Texaco Incorporated
S. T. Hadden, Monsanto Company, Hydrocarbons Division (retired)
D. L. Camin, Chairman, Sun Oil Company

PREFACE

In 1942, the American Petroleum Institute established the 44th of a series of basic research projects in the area of chemistry and properties of petroleum under the direction of Dr. Frederick D. Rossini, Chief of the Thermochemistry Section of the National Bureau of Standards, Washington, D. C. The mandate of this new American Petroleum Institute Research Project 44 was to serve as a central agency for collecting, calculating, critically selecting, and compiling numerical data on the physical and thermodynamic properties of hydrocarbons and certain classes of related non-hydrocarbon compounds. Those 'selected' or 'critical' data were to be issued in table form for ready use by the laboratories of the petroleum industry. As a result of the exigencies of World War II, a rather unique data compilation and theoretical correlation organization was founded by a segment of the U. S. private industry to compile high-quality standard reference data on pure substances to meet the needs of science and technology, not only in the United States but throughout the world.

One of the desirable criteria of a critical or standard reference data compilation effort is the rapid dissemination of the information in a form convenient for revision of old data and addition of new data. A loose-leaf sheet format was adopted whereby data on physical, thermodynamic, and, at a later date, spectral (infrared, ultraviolet, Raman, mass, and nuclear magnetic resonance) properties of hydrocarbons and related compounds could be printed and rapidly distributed in supplementary lots or volumes to interested industrial, academic, and government scientists and engineers.

The usefulness and importance of the six data publications, namely, the numerical tables and the five spectral catalogs, published by the API Research Project 44 under the title "Selected Values of Properties of Hydrocarbons and Related Compounds" may be described briefly as follows:

- data on physical properties help research laboratories and refineries to identify petroleum fractions as well as pure compounds
- data on thermodynamic properties permit reliable calculations of heat balances and evaluations of chemical equilibria to improve chemical process design and operation carried on by chemical and petroleum industries
- data on spectral properties help in making rapid analyses of plant streams and product materials in the refining processes, as well as in identifying individual compounds.

To further meet the specific needs of the working scientist and engineer, hard-cover bound volumes of the API Research Project 44 tables were made available from time to time such as the 'green' volume at the National Bureau of Standards, Washington, D. C. in 1947 (F. D. Rossini, K. S. Pitzer, W. D. Taylor, J. P. Ebert, J. E. Kilpatrick, C. W. Beckett, M. G. Williams, and H. C. Werner, NBS Circular C461, U. S. Govt. Printing Office, Washington, D. C., 1947, 483 pp.). Six years later, at the new location at Carnegie Institute of Technology, Pittsburgh, the 'red' volume appeared (F. D. Rossini, K. S. Pitzer, R. L. Arnett, R. M. Braun, and G. C. Pimentel, Carnegie Press, Carnegie Institute of Technology, Pittsburgh, Pennsylvania, 1953, 1050 pp.). The principal publications of the API Research Project 44 tables in the form of loose-leaf data sheets continued to be published to meet the most demanding requirements for high quality data, whereas, the bound volumes, as typical handbooks, served the engineer who had an on-the-spot need for reliable data but did not require the newest or the most recently revised information of highest accuracy.

When the API Research Project 44 was transferred to Texas in 1961, under the direction of Professor Bruno J. Zwolinski, to become affiliated with the Thermodynamics Research Center of Texas A&M University, consideration was given to publishing a third bound edition of the API 44 tables to replace the red 1953 edition which was out-of-print and out-of-date. At that time the number of valid sheets on physical and thermodynamic properties numbered well over 2000 and would have required at least three massive volumes. The contemplated new bound publication would have become a rather formidable standard reference work suitable for libraries but it would have failed to serve the immediate needs of the individual working scientist, the engineer, or even the student at a desk or in the laboratory. Furthermore, over a period of several years, our TRC Data Distribution Office frequently received requests from recipients for small volumes of data on specific properties such as vapor pressures, heats of combustion, PVT data, etc. or, alternatively, on certain properties for a closely related group of compounds, such as the alkanes, the aromatics, or the unsaturated hydrocarbons. After consideration of these factors together with the advice and cooperation of the Advisory Committee of the API Research Project 44, a decision was reached late in the sixties to embark on a new series of small, convenient data handbooks based on the principal tables of selected properties of the API Research Project 44.

This current compilation entitled, "Handbook of Vapor Pressures and Heats of Vaporization of Hydrocarbons and Related Compounds," represents the first in the new series of API 44—TRC Publications in Science and Engineering. We hope that these concise data handbooks will serve the needs of the working scientist, engineer, and student at the laboratory bench, research desk, or even at the conference table.

The reliability of physicochemical property data is directly a function of the precision and accuracy of measurement by experienced investigators on samples of selected 'key' compounds of certified purity. For this reason the API Research hydrocarbons and the API Sulfur samples that have served as sources of boiling point and vapor pressure data for the tables are delineated in Section V of this handbook.

A data compilation publication is seldom the effort of a single individual but is born of the cooperative interest and effort of a group of highly motivated and experienced scientists, or data 'compilers', in the current terminology. This is particularly true of the American Petroleum Institute Research Project 44. For the last twenty-nine years, this project has continuously generated critical data on substances at four locations, namely, the National Bureau of Standards (1942-1950), Carnegie Institute of Technology (1950-1961), University of California, Berkeley (1946-1951), and currently, at Texas A&M University (1961-). The problem of acknowledging contributions and thanking contributors is a most difficult one because of the vast number of people involved. This compilation is the result of the cooperation of hundreds of chemists, engineers, physicists, literature information specialists, data programmers and computer specialists, editorial and composition experts, and many, many undergraduate, graduate, and postdoctoral students at the four locations of the API Research Project 44 for over a quarter of a century. The authors feel most humble in acknowledging the many outstanding contributions of all these past and current staff members of the Project together with the many notable individuals from industry who served as members of the Advisory Committees for the API Research Project 44 over the years. The echoes of their footsteps have not died in the halls of science.

Notification of errors that will no doubt be discovered by critics and users of this handbook will be gratefully received by the authors so that a corrected and improved version may be issued at a later date.

College Station, Texas, U. S. A. June, 1971

Bruno J. Zwolinski Director American Petroleum Institute Research Project 44

INTRODUCTION

This handbook has been compiled for the convenience of those who are concerned with the vapor-liquid equilibrium phenomena of compounds of importance in the refining of petroleum and the manufacture of petrochemicals. The numerical data on the boiling points, vapor pressures, and heats of vaporization of pure hydrocarbons and certain related sulfur compounds contained in the handbook have been extracted from "Selected Values of Properties of Hydrocarbons and Related Compounds," a publication of the American Petroleum Institute Research Project 44 of the Thermodynamics Research Center, Texas A&M University, College Station, Texas (Loose-leaf data sheets, extant, 1971).* The data are organized into the following six sections.

Section I. Tables of Boiling Points in Degrees Celsius at Designated Pressures from 10 mm to 1500 mmHg. These are the "k-tables" reprinted from APIRP 44 Tables and arranged in table number order.

Section II. Tables of Vapor Pressure in Pounds per Square Inch (absolute) at Designated Temperatures in Degrees Fahrenheit in the Range from 0.2 to 30 lb in⁻². These are the "k-E-tables" reprinted from the APIRP 44 Tables and arranged in table number order. Each k-table has a corresponding k-E-table (except for water and the alkyl anthracenes and phenanthrenes).

Section III. Tables of the Normal Boiling Points, Heats of Vaporization, and Related Data in Various Convenient Units. These numerical data are derived from the values in the k-, k-E-, and m-tables of the APIRP 44 Tables, supplemented in some cases from the data files of the Thermodynamics Research Center. The compounds are arranged according to classes on the basis of unsaturation or C/H ratio in a manner similar to the table number order for the hydrocarbons and the sulfur compounds, respectively. This table also serves as a compound index to the tables of boiling points and vapor pressures.

Section IV. Index of Compounds by the Order of their Normal Boiling Points. This index lists all compounds from the k- and k-E-tables with their respective normal boiling point values in °C and °F and gives page numbers of both the k- and k-E-tables where complete vapor pressure data are located for each compound. Some additional compounds of technological importance extracted from the a-tables of the APIRP 44 Tables are listed that are not included in the k- or k-E-tables. A separate list of boiling points at 10 mm is given for those compounds whose boiling point is not known or is not measurable at one atmosphere.

Section V. Summary of Precision Vapor Pressure Studies on API Research Hydrocarbons and API Standard Sulfur Samples.

Section VI. Name Index of Compounds (CA listing as in the API 44-TRC Comprehensive Index). The data reported in the handbook are based on a selection of the "best" experimental measurements available. In some cases, where experimental data are not available, the tabulated values are calculated from an empirical correlation or an extrapolation. The sources of the values are identified in the appropriate Specific References sheets for the a-, k- and k-E-, and m-tables of the principal APIRP 44 Tables. The initial date printed below the title at the top of each of the k- and k-E-tables represents the date that the table was first issued in the parent APIRP 44 Tables. Subsequent dates show when the table was reissued due to revision or correction. Dates of corrected sheets are enclosed in parentheses. Tables having the same final date are internally consistent. The most recent date of revision indicates the extent of the literature search for the data appropriate to that table.

The uncertainties in the tabulated values are indicated by the number of significant figures reported. The range of estimated uncertainties in the variables and properties listed is given in the following table:

		When the valu	ie is written to	>
Property	1.	0.1	0.01	0.001
	•	the uncertainty	is estimated to be	
Temperature	2. to 20.	0.2 to 2.	0.02 to 0.2	0.002 to 0.02
Pressure	2. to 10.	0.2 to 2.	0.02 to 0.2	0.002 to 0.02
Enthalpy	4. to 10.	0.4 to 4.	0.04 to 0.4	0.004 to 0.04

^{*}Hereafter abbreviated to APIRP 44 Tables.

In many cases the uncertainties in the relative values of a series of numbers are appreciably less than the uncertainties in each individual number. This is generally true for a series of vapor pressures at various temperatures or a series of boiling points at various pressures for the same compound, or for a series of values of the same property for the members of a homologous series of compounds.

The definition of symbols used in the equations and tables of this book are:

Symbol	Definition
A, B , and C	Parameters in the Antoine equation for vapor pressure
β	Second virial coefficient
C_p	Heat capacity per mole at constant pressure
H	Enthalpy (per mole, unless otherwise indicated) equals $E + PV$
ΔH_{v}	Heat (enthalpy) of vaporization, the enthalpy of the real gas in equilibrium with a solid or liquid minus the enthalpy of the same quantity of solid or liquid
P	Pressure, also the vapor pressure of a gas phase in equilibrium with a condensed phase
R	Gas constant
$t^{-\frac{4}{3}}$	Temperature, °C (Celsius)
t_b	Boiling point, °C
T	Temperature, K (kelvins)
T_b	Boiling point, K
V	Volume (per mole, unless otherwise indicated)
ΔV_{v}	Volume of a real gas in equilibrium with a solid or liquid minus the volume of the same quantity of solid or liquid

The vapor pressures and boiling points reported in the k- and k-E-tables have been calculated primarily from the Antoine equation (see C. Antoine, C. R. Acad. Sci. 107, 681 (1888)).

$$\log_{10}P = A - \frac{B}{C+t} \tag{1}$$

The only exceptions occur in the k-tables for some of the alkyl naphthalenes, anthracenes, phenanthrenes and sulfur compounds where the data are not of sufficient precision to determine the Antoine constants for some compounds. Our experience has demonstrated the convenience and effectiveness of the Antoine equation in smoothing precise vapor pressure data on a variety of hydrocarbons well within the experimental uncertainty in the defined range of 10 mm to 1500 mmHg. The representation of vapor pressures over a wider range of pressures, however, may require the use of a more complex equation of four or more parameters. In some instances it has proved convenient to use two or more sets of Antoine constants for wider ranges of temperature or pressure (see tables 2-1-(1.01) and 2-1-(1.02) for water).

The Antoine parameters A, B, and C, based on the same regression procedure, are characteristic of each individual compound. They have been obtained either by fitting the Antoine equation to the experimental vapor pressures and boiling points or by the application of empirical correlation procedures as described by Rossini, Mair, and Streiff ("Hydrocarbons from Petroleum, an Account of the Work of the APIRP 6," Reinhold Publishing Company, New York, New York, 1953) and Kreglewski and Zwolinski (Rocz. Chem. 35, 1041, 1059 (1961)). G. W. Thomson (Chem. Rev. 38, 1 (1946); "Physical Methods of Organic Chemistry," edited by A. Weissberger, Vol. 1, Part I, 2nd edition, Interscience Publishers, Inc., New York, New York, 1949) has also reviewed the applications of the Antoine equation and other equations and has described graphical and numerical methods for calculating the parameters. When accurate experimental data are available, a numerical least-squares fitting procedure is preferable. According to the Antoine equation, pressure taken directly as a function of temperature is nonlinear in the parameters A, B, and C. The values reported in the recently revised tables for the normal alkanes, C₁ to C₂₀ [table 23-2-(1.101)-k and -k-E] and the isomeric alkanes C₁ to C₅ [table 23-2-(1.200)-k and -k-E] were obtained by a nonlinear least-squares technique using appropriately weighted values of experimental vapor pressure and heat of vaporization data. However, most of the tabulated data are based on the least-squares technique of

C. B. Willingham, W. J. Taylor, J. M. Pignocco and F. D. Rossini, J. Res. Nat. Bur. Stand. 35, 219 (1945). Equation (1) can be transformed to

$$t \log P = (AC - B) + At - C \log P \tag{2}$$

Here the term $t \log P$ can be considered as a function of the independent variables t and $\log P$. The constants (AC - B), A and C can then be calculated directly by the usual linear least-squares technique, and the value of B can be calculated from these.

If the constant, C, equals 273.15, the Antoine equation reduces to the familiar integrated form of the Clausius-Clapeyron equation for an ideal gas with constant heat of vaporization, namely, the Kelvin equation,

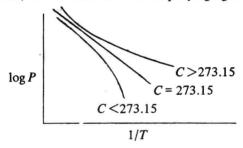
$$\log P = A - B/T \tag{3}$$

According to equation (3) $\log P$ is a linear function of 1/T, with the slope of -B. The first and second derivatives of $\log P$ with respect to 1/T can be calculated from equation (1).

$$\frac{d \log P}{d(1/T)} = -B \left(\frac{t + 273.15}{t + C} \right)^2 \tag{4}$$

$$\frac{d^2 \log P}{d(1/T)^2} = 2B(C - 273.15) \left(\frac{t + 273.15}{t + C}\right)^3$$
 (5)

If C is greater than 273.15 the $\log P - 1/T$ plot has positive curvature, and if C is less than 273.15, the $\log P - 1/T$ plot has a negative curvature, as illustrated in the accompanying figure.



The values of A, B, and C obtained by fitting the Antoine equation to experimental data should be interpreted with care, especially if they are to be used for extrapolating outside the experimental range or for developing correlations with other properties or with molecular structure. In structural correlations, the Antoine constants should be defined by the same curve fitting procedure. The effect of varying C on the deviations between calculated and observed vapor pressures is small when A and B are simultaneously adjusted to obtain the best fit. As a result, the C parameter is not usually well-determined by the data. The uncertainty in C depends on the accuracy of the original pressure and temperature data, on the range of data used in the fitting calculation, and on the manner of its distribution over this range. A minimum of three pairs of temperature-pressure values are required to determine the three Antoine parameters. The uncertainty in the parameter C can be simply illustrated by considering the effect of experimental errors on the value of C calculated from three such pairs of values. Let the three pressures be designated as P_1, P_2 , and P_3 , where P_1 is the lowest pressure; P_3 , the highest pressure; and $P_2 = (P_1 P_3)^{1/2}$. Assume that the experimental uncertainty is expressed in terms of the uncertainty in temperature and that all three temperatures have the same uncertainty. The ratios of the uncertainty in C, δC , to the corresponding uncertainty in t, δt , where the uncertainties are considered as proportional to the respective standard deviations, are shown in the following table for several typical values of P_1 , P_3 , and A. For example, the uncertainty in the value of C calculated from boiling points at 10, 32, and 100 mm that are uncertain by one degree is 61.2°C when A equals 5. Although additional data points will help to reduce the uncertainties in the parameters, it is clear that a meaningful value of C can be obtained only when accurate data are available over a wide range of pressures. When this condition is not fulfilled, it is better to calculate C from a correlation procedure or to estimate it by comparison with similar compounds, and then calculate A and B from the available data.

Uncertainties in the Antoine C Constant Calculated From Three Data Points

P_1 , mm	<i>P</i> ₃ , mm	A = 5	A = 6	A = 7
			Values of $\delta C/\delta t$	
10	100	61.2	100.4	149.4
10 100	1000 1000	12.2 31.8	20.8 61.2	31.8 100.4
200	400	350	668	1112

The Antoine C parameter is always less than 273 for organic compounds below 1500 mm. In general, it is smaller for compounds having a high boiling point, and it decreases for any homologous series of compounds as the boiling point increases. Larger values of C are required for higher pressure ranges, and apparently C approaches the critical temperature for vapor pressures in the vicinity of the critical point. In the Report of Investigation of the Manufacturing Chemists Association of November 30, 1960, "New Methods of Calculation of Some Physical Properties of Liquids Based on the Antoine Equation. I. General," A. Kreglewski and B. J. Zwolinski describe several useful correlation procedures. The equations

$$C = 273.2 + 0.013 \ \Delta C_p \ T_b \tag{6}$$

and

$$C = 273.2 - 0.04 T_b - 3 \times 10^{-3} T_b^2$$
 (7)

reproduce the C parameter for nonpolar nonconducting liquids within a few degrees. ΔC_p is the heat capacity of the gas minus that of the liquid in cal K⁻¹ mol⁻¹ and T_b is the normal boiling point in K. Additional correlation procedures by the same authors are described in the Report of Investigation of the Manufacturing Chemists Association of August 15, 1965, "New Methods of Calculation of Some Physical Properties of Liquids Based on the Antoine Equation II. n-Alkanes and n-Alkyl Compounds." A. P. Kudchadker and B. J. Zwolinski, J. Chem. Eng. Data, 11, 253 (1966) obtained the equation

$$C = 273.15 - 4.49159 \times 10^{-2} T_b - 2.68408 \times 10^{-4} T_b^2 - 5.18608 \times 10^{-8} T_b^3$$
 (8)

by a least-squares fit to the C parameter of the n-alkanes from C_3 to C_{17} .

When an orderly arrangement of data becomes available on closely related groups of compounds, many a chemist and chemical engineer becomes highly motivated to a reanalysis and additional structural correlation of the reported data. This may be commendable; however, one should have a clear understanding that only smoothed and correlated data are reported in this handbook. Correlations based on correlated data are not recommended. Such investigators should consult the Specific References sheets of the original APIRP 44 publications to determine which of the reported values are smoothed experimental data and which values have been arrived at by precision-reliable correlation procedures.

The derivative of the vapor pressure with respect to temperature is related to the heat of vaporization and the volume change on vaporization by the well-known thermodynamic relation

$$\frac{dP}{dT} = \frac{\Delta H_{\nu}}{T \Delta V_{\nu}} \tag{9}$$

From equation (1) the temperature derivative of the vapor pressure is found to be

$$\frac{dP}{dT} = \frac{2.303 BP}{(C+t)^2} \tag{10}$$

If the volume of one mole of the gas in equilibrium with the condensed phase can be adequately represented by the virial equation with two terms,

$$V^{g} = RT/P + \beta \tag{11}$$

then the heat of vaporization can be calculated from the Antoine parameters B and C and the second virial coefficient.

$$\Delta H_{\nu} = \frac{2.303 \, BPT}{(C+t)^2} \left[RT/P + \beta - V \right] = \frac{B \, T}{(C+t)^2} \left[4.576 \, T + 7.337 \, (\beta - V) \, P \right] \tag{12}$$

where V is the molar volume of the condensed phase. In the expression on the right side of equation (12) β and V are in units of cm³ mol⁻¹, P in mmHg and ΔH_{ν} in kcal mol⁻¹. Equation (12) can also be used to help establish the values of B and C from calorimetric values of heats of vaporization.

Since 1960 the International Bureau of Weights and Measures has recommended the use of the International System of Units (SI) for scientific and technical work. The pertinent SI units and their definitions are listed below.

Basic SI Units

Quantity	Name	Symbol	Definition
length	meter	m	the length of 1,650,763.73 wavelengths in vacuum of the radiation corresponding to the transition between the levels $2p_{10}$ and $5d_5$ of krypton-86
mass	kilogram	kg	the mass of the international prototype kilogram
thermodynamic temperature	kelvin	K	1/273.16 of the thermodynamic temperature of the triple point of water
time	second	S	the duration of 9,192,631,770 periods of the radiation corresponding to the transition between the two hyperfine levels of the ground state of cesium-133
amount of substance	mole	mol	the amount of substance of a system which contains as many elementary entries as there are atoms in 0.012 kilograms of carbon-12

Derived SI Units

Quantity	Name	Symbol	Relation to Basic SI Units
force	newton	N	kg m s ⁻²
pressure	pascal	Pa	N m ⁻²
pressure	bar	bar	10 ⁵ N m ⁻²
mass	gram	g	10 ⁻³ kg
length	centimeter	cm	10 ⁻² m
length	millimeter	mm	10 ⁻³ m
energy	joule	J	kg m ² s ⁻²
energy	kilojoule	kJ	1000 J

Other Units Defined in Terms of SI Units

Quantity	Name	Symbol	Definition
length	inch	in	$2.54 \times 10^{-2} \text{ m}$
mass	pound	lb	0.45350237 kg
force	kilogram-force	kgf	9.80665 N
pressure	atmosphere	atm	101325 N m ⁻²
pressure	millimeter of mercury	mmHg*	133.3224 N m ⁻²
energy	kilowatt-hour	kwh	$3.6 \times 10^6 \text{ J}$
energy	thermochemical calorie	cal	4.184 J
energy	I. T. calorie	cal _{IT}	4.1868 J

^{*}Numerically nearly identical to the torr.

Pressures are reported in units of mmHg in the k-tables and in units of pounds (force) per square inch in the k-E-tables. Heats of vaporization are reported in units of kilojoules and thermochemical kilocalories per mole, in thermochemical calories per gram, and I. T. Btu per pound in the table of Section III. In those tables bearing the final date up through April 30, 1969, temperatures are reported in terms of the International Practical Temperature Scale of 1948 (IPTS-48), or the equivalent on the Fahrenheit scale according to the relation

$$t(^{\circ}F) = (9/5) t (^{\circ}C) + 32$$
 (13)

In those tables which are dated October 31, 1969 or later, both revised and corrected data sheets, the temperatures are reported on the International Practical Temperature Scale of 1968 (IPTS-68). A footnote indicating the use of the new scale is included in all of these tables. The International Practical Temperature Scale of 1968 is described in *Metrologia*, 5, 35 (1969), and a table of differences between the IPTS-68 and IPTS-48 for the range of temperatures of concern here is included among the following tables.

UNITS OF SPECIFIC ENERGY

	joule ⁻¹	cal g ⁻¹	I.T. cal g ⁻¹	I:T. Btu lb-1	kilowatt-hr lb ⁻¹
1 joule g ⁻¹	1	0.2390057	0.2388459	0.4299226	1.259979 X 10 ⁻⁴
1 cal g'	4.184	1	0.9993312	1.798796	5.271752 × 10 ⁻⁴
1 I.T. cal g ⁻¹	4.1868	1.000669	1	1.8	5.275279 × 10 ⁻⁴
1 I.T. Btu lb ⁻¹	2.326	0.5559273	0.555555	1	2.390711 × 10 ⁻⁴
1 kilowatt-hr lb ⁻¹	7936.641	1896.903	1895.643	3414.425	1

Comparison of the International Practical Temperature Scales of 1948 and 1968

t	IPT	S-6	8)	-	t(IP	Т	S-4	(8)
	-	9	•				9	

t_{68} °C	-0	-10	-20	-30	-4 0	-50	-60	-70	-80	-90	-100
-100	0.022	0.013	0.003	-0.006	-0.013	-0.013	-0.005	0.007	0.012		
-0	0.000	0.006	0.012	0.018	0.024	0.029	0.032	0.034	0.033	0.029	0.022
t_{68} °C	0	10	20	30	40	50	60	70	80 °	90	100
0	0.000	-0.004	-0.007	-0.009	-0.010	-0.010	-0.010	-0.008	-0.006	-0.003	0.000
100	0.000	0.004	0.007	0.012	0.016	0.020	0.025	0.029	0.034	0.038	0.043
200	0.043	0.047	0.051	0.054	0.058	0.061	0.064	0.067	0.069	0.071	0.073
300	0.073	0.074	0.075	0.076	0.077	0.077	0.077	0.077	0.077	0.076	0.076

Values of the Gas Constant, R, in Various Units

8.31434 J K⁻¹ mol⁻¹

1.98717 cal K-1 mol-1

1.98585 I.T. cal K-1 mol-1

82.0562 cm3 atm K-1 mol-1

0.082056 liter atm K-1 mol-1

62,362.7 cm3 mmHg K-1 mol-1

10.8059 ft3 lb in-2 F-1 lb-mol-1

1.98585 I.T. Btu F-1 lb-mol-1

If A, B, and C are the parameters in the Antoine equation (equation (1)) in which P is in mmHg and t in degrees Celsius and A', B', and C' are corresponding parameters for P in 1b in $^{-2}$ and t in degrees Fahrenheit, the two sets of values are related by

$$A' = A - 1.71362$$

B' = 1.8 B

C' = 1.8 C - 32.

UNITS OF MASS

	50	kg	ZO	lb	metric ton	ton
1 gram	1	10-3	0.03527396	2.204623×10^{-3}	9−01	1.102311×10^{-6}
1 kilogram	1000.	-	335.27396	2.204623	10-3	1.102311×10^{-3}
1 ounce (avdp)	28.34952	0.02834952	-	0.0625	2.834952 × 10 ⁻⁵	3.125×10^{-5}
1 pound (avdp)	453.5924	0.4535924	16.		4.535924 × 10 ⁻⁴	5. × 10 ⁻⁴
1 metric ton	106	1000.	35273.96	2204.623	_	1.102311
1 ton	907184.7	907.1847	32000.	2000.	0.9071847	1.

UNITS OF PRESSURE

3	dyne cm ⁻²	N m -2	atm	kgf cm ⁻²	mmHg (torr)	in Hg	lb in ⁻²
1 dyne cm ⁻²	1	0.1	9.869233×10^{-7}	1.019716 × 10 ⁻⁶	7.500617 × 10 ⁻⁴	2.952999 X 10 ⁻⁵	1.450377×10^{-5}
1 N m-2	10.	-	9.869233 X 10 ⁻⁶	1.019716 X 10 ⁻⁵	7.500617×10^{-3}	2.952999 X 10 ⁻⁴	1.450377 × 10 ⁻⁴
1 atm	1013250.	101325.0	1	1.033227	760.	29.92126	14.69595
1 kgf cm ⁻²	980665.	98066.5	0.9678411	_	735.5592	28.95903	14.22334
1 mmHg	1333.224	133.3224	1.3157895×10^{-3}	1.3595099 X 10 ⁻³	-	0.03937008	0.01933678
1 in Hg	33863.88	3386.388	0.03342105	0.03453155	25.4	1	0.4911541
1 lb in -2	68947.57	6894.757	0.06804596	0.07030696	51.71493	2.036021	1

UNITS OF ENERGY

	joule	cal	I.T cal	I.T. Btu	kilowatt-hr	liter-atm	ft³ lb in⁻²
l joule	-	0.2390057	0.2388459	9.478172 × 10 ⁻⁴	9.478172 × 10 ⁻⁴ 2.7777 × 10 ⁻⁷	9.869233×10^{-3}	5.121960×10^{-3}
	4.184		0.9993312	3.965667×10^{-3}	$3.965667 \times 10^{-3} \mid 1.1622 \times 10^{-6} \mid$	0.04129287	0.02143028
I.T. cal	4.1868	1.000669	_	$3.968321 \times 10^{-3} \mid 1.163000 \times 10^{-6}$	1.163000 × 10 ⁻⁶	0.04132050	0.02144462
I.T. Btu	1055.056	252.1644	251.9958	-	2.930711 × 10 ⁻⁴	10.41259	5.403953
kilowatt-hr	3600000	860420.7	859845.2	3412.142	_	35529.24	18439.06
liter-atm	101.3250	24.21726	24.20106	0.09603757	2.814583×10^{-5}	1	0.5189825
1 ft³ lb in-2	195.3278	46.66295	46.63174	0.1850497	5.423272×10^{-5}	1.926847	-

Section I. Tables of Boiling Points in Degrees Celsius at Designated Pressures from 10 to 1500 mmHg

These tables are taken from the following supplementary volumes to "Selected Values of Properties of Hydrocarbons and Related Compounds:"

Supplementary Volume 25, dated December 31, 1952
Supplementary Volume 26, dated October 31, 1953
Supplementary Volume 27, dated April 30, 1954
Supplementary Volume 29, dated April 30, 1955
Supplementary Volume 40, dated October 31, 1960
Supplementary Volume 41, dated April 30, 1961
Supplementary Volume 42, dated October 31, 1961
Supplementary Volume 47, dated October 31, 1964
Supplementary Volume 49, dated April 30, 1966
Supplementary Volume 50, dated October 31, 1966
Supplementary Volume 52, dated October 31, 1967
Supplementary Volume 55, dated April 30, 1969
Supplementary Volume 56, dated October 31, 1969
Supplementary Volume 57, dated April 30, 1970
Supplementary Volume 58, dated October 31, 1970