GERG TECHNICAL MONOGRAPH NO. TPC/1 (1986)

presented at

INTERNATIONAL GAS RESEARCH CONFERENCE
Toronto, 8-11 September 1986

SOME THERMOPHYSICAL CONSTANTS OF COMPONENTS OF NATURAL GAS AND COGNATE FLUIDS

CONSTANTES THERMOPHYSIQUES DES COMPOSANTS DE GAZ NATUREL ET DES FLUIDES APPARENTES

compiled by

A E HUMPHREYS

British Gas Corporation Research & Development Division
London Research Station, Michael Road, London SW6, U.K.

on behalf of

The Thermodynamics Research Committee
GROUPE EUROPEEN DE RECHERCHES GAZIERES (GERG)

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CONTENTS

ABSTRACT

This booklet gives tabulations of numerical values of a set of thermophysical constants and properties for over 50 pure molecular species typically found in natural gas or in related fluid mixtures, such as those encountered in natural gas processing, the production of substitute (synthetic) natural gas, and in gas characterisation. Source references, means of derivation and contextual commentary, often given rather skimpily in documents of this sort, are given here in some detail. The complete set of values has been prepared as a collaborative effort by the Thermodynamics Research Committee of G.E.R.G., and is intended to form a sort of informal European standard. An introductory abbreviated version of this document was published in the proceedings of the 1986 International Gas Research Conference held in Toronto, but space limitations prevented the publication there of this full version.

RÉSUMÉ

Ce livret donne les tableaux des données numériques d'un ensemble des constantes et propriétés thermophysiques de plus de 50 espèces moléculaires purs que l'on trouve typiquement dans le gaz naturel ou dans les mélanges fluides apparentés, tels que ceux recontrés dans le traitement du gaz naturel, la production de gaz naturel de substitution (gaz de synthèse), et dans la caractèrisation des gaz. Les sources des références, les moyens de dérivation et les commentaires sur le contexte qui, dans les documents de ce genre sont donnés souvent d'une façon plutôt brève, sont fournis en détails dans ce livret. L'ensemble complet des données résulte d'un travail de collaboration du comité de recherche "propriétés thermodynamiques" du G.E.R.G. et a vacation à constituer une sorte de norme européenne. Une version d'introduction abrégée de ce document fut publiée dans la rapport du Congrès International de la Recherche Gazière 1986 qui eu lieu à Toronto, mais les limitations d'espace empêchèrent la publication de la version complète dans ce rapport.

FOREWORD

The Groupe Européen de Recherches Gazières or, as it is more colloquially known, GERG, is an association of European gas utilities which meets for the purposes of exchanging information on research topics of common interest and of contributing sets of research results into a common pool for mutual benefit. Currently the membership of G.E.R.G. comprises A.R.G.B. (Belgium), Gaz de France (France), Ruhrgas (Federal Republic of Germany), Italgas (Italy), the VEG-Gasinstituut (Netherlands) and British Gas (United Kingdom) as the official national members, but with strong involvement in technical activities of the group from Distrigaz (Belgium), S.N.A.M. (Italy) and Gasunie (Netherlands). G.E.R.G. activities date from 1961, becoming formalised in 1965.

The Thermodynamics Research Committee, more precisely the G.E.R.G. Committee on the Thermodynamic Properties of Natural Gases, was formed within this framework in 1971 with the aim of co-ordinating approaches to common problems involving the application of thermophysical knowledge. Relevant topics for study arise from many areas of gas industry operations. Some aspects of the Committee's past and continuing work have been discussed elsewhere [1]. The chairmanship of the G.E.R.G. Thermodynamics Committee is held by British Gas.

The present document clearly owes its origin to the natural wish (and need) within any such group to carry out its tasks on a uniform and agreed basis, a most fundamental aspect of which concerns pure component thermophysical constants and properties. In that sense the total compilation forms a sort of internal, informal European gas industries standard; wider currency would have obvious benefits.

INTRODUCTION

Because of the prospect of increasing international trade (custody transfer) of natural gas amongst the G.E.R.G. member countries, as well as for other reasons relating to the mutual interests of the European gas industries, it is important that there be a substantial (preferably complete) measure of agreement about how best to determine the relevant thermophysical properties of pipeline quality gas and other fluids. Specialised instruments, notably recording calorimeters, play their part in this, but increasingly it is a compositional analysis (made invariably by gas chromatography) that is the more readily and generally available, and from which the mixture properties must be inferred. The negative aspect of this is the consequent need to have an international standard calculational method (recipe) of acceptable accuracy for the prediction of each property of interest from composition, but on the positive side it does open up the possibility that - given enough thermodynamically consistent recipes - a whole range of otherwise more or less inaccessible properties can be predicted [2].

Even given such recipes, there is one further and most fundamental aspect, viz. what are the best values for the thermophysical constants (e.g. critical temperatures and pressures), or variable properties at fixed conditions (e.g. compressibility factors), of the individual components, that are in some way to be combined by the recipes? That is the question which is addressed here.

This booklet presents a compilation of such pure component constants and properties prepared as a collaborative effort by the G.E.R.G. Thermodynamics Research Committee. Previously, no such compilation enjoyed widespread currency within Europe, although to some extent the present set of values supersedes a much more restricted set published at the 1973 World Gas Conference (held in Nice) by Lorenz [126]. In general, each country's gas industry formerly used its own "preferred" values, a situation which was aided, abetted and obscured by the fact that the legal "standard" metrological condition at which some properties are defined (notably calorific values) varies from country to country; these standard conditions have not generally changed, but values referring to the different conditions have now been made mutually consistent.

SUMMARY OF CONTENTS

The physical constants and properties given for each distinct molecular species are as follows:

- Table 1: Simple Physical Properties
    - Relative Molecular Mass (Molecular Weight)
    - Normal (Atmospheric) Melting Temperature (or Triple Point Temperature and Pressure)
    - Normal (Atmospheric) Boiling Temperature (or Sublimation Temperature)
- Table 2: Critical Properties
    - Critical Temperature
    - Critical Pressure
    - Critical Density
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- Table 3: Standard Volumetric Properties
    - Compressibility Factor (a) 0°C, 1.01325 bar
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    - Second Virial Coefficient at 15°C
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- Table 4: Enthalpies of Formation and Combustion
    - Standard Enthalpy of Formation at 25°C
    - Standard Enthalpy of Combustion (a) 25°C
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        (c) 0°C, 1.01325 bar
- Table 5: Calorific Values
    - Ideal Gas Gross Calorific Value (volume basis) (a) 25/0°C
        (b) 15/0°C
        (c) 15/15°C
    - Real-Gas Gross Calorific Value (volume basis) (a) 25/0°C, 1.01325 bar
        (b) 15/0°C, 1.01325 bar
        (c) 15/15°C, 1.01325 bar
    - (mass basis) (d) 25°C, 1.01325 bar
- Table 6: Flammability Data
    - Lower Flammability Limit in Air
    - Upper Flammability Limit in Air
    - Minimum Autoignition Temperature.

This compilation interprets the phrase "components of natural gas and cognate fluids" in a liberal fashion. Many of the over 50 species for which constants are given would never be found in natural gas proper, but can be important trace components of, for example, a substitute (synthetic) natural gas process stream, or are perhaps used in natural gas processing or characterisation.

For each property a derivation and/or source reference is given. Most of the source references are in fact themselves internationally respected data compilations of one sort or another; without at this point "decoding" the various organisational acronyms, let us just stress that it has not been our intention to compete with or repeat work carried out by, for example, API, CODATA, DIPPR, ESDU, GPA, ISO, IUPAC, NBS, NPL, PPDS or TRC (to "name" just some!), simply to select the "best" from their compilations wherever appropriate.

Considerable contextual commentary, often given rather skimpily in documents of this sort, is given to accompany the compilation. This is particularly so in discussions of derived, as opposed to selected, values; a special effort has been made to assure internal (thermodynamic) consistency of all values. One particular document with which we especially hope to achieve external consistency is the forthcoming revision of International Standard ISO 6976 [3], which is concerned with the calculation from composition of calorific value and related quantities.

Units are metric, generally Système International (SI), throughout.

SOURCE LITERATURE

The source literature for each numerical value in the tabulations (except for those values which are derived from other tabulated values by some method prescribed elsewhere in the commentary) is identified by a 3-letter quasi-mnemonic or acronym. The intention is that most of these will soon become more readily familiar to the user than would an equivalent set of reference numbers - which would also serve to "confuse" the tables. However, the alphabetically-ordered tabular references do also have code numbers (starting at 101) in order that they can be referred to in the normal way in the main text.

There is one slight exception to the "3-letter identifier" rule. This is for the case of the very frequent citations to values taken from the highly respected tabulations published by the Thermodynamics Research Center at Texas A & M University. Because these tabulations are the subject of regular updates, a 2-digit number identifying the date of the table referred to is appended to the basic "TRC" code, i.e. TRC.85 refers to information published in 1985 as part of either the TRC Thermodynamic Tables (Hydrocarbons) or the very closely allied TRC Thermodynamic Tables (Non-Hydrocarbons)[145].

Of course, it is often the case that any one of several "good quality" (secondary) sources could be used with equal correctness to refer to the selected value of a particular quantity. In such cases the choice of citation has been made somewhat arbitrarily, but nevertheless with a view to international visibility and respect - although that again introduces an element of subjective judgement. There is no absolute "pecking order". The usual tendency is to cite a more property-specific or compound-specific secondary compilation or review in preference to a more general compilation. Citation to primary literature, especially if this has not been subjected to independent critical evaluation and/or does not come from a scientist or laboratory of established high reputation, is used sparingly.

IMPLIED ACCURACY

It is difficult (and impracticably costly in space) to give a worthwhile accuracy statement for each individual figure listed in the tabulations. Instead of attempting this, the general intention (i.e. the guiding principle) is that the uncertainty in any value should be in the last quoted digit; thus, the penultimate digit (after rounding) should be significant. However, the usual (though not invariable) practice adopted is to quote values from a source to the same number of digits as the source (some care is needed here if a conversion of units has to be performed on the source value before its inclusion in a table).

Usually principle and practice correspond well (in general, if the authors of source literature have quoted "responsibly" by retaining one semi-redundant digit, perhaps as an aid to interpolation).

It is, nevertheless, not universally the case in the present tabulations that practice matches principle. For example, in Table 2 the third decimal place for the acentric factor is not always significant, nor, in Table 4, is the first decimal place for the standard enthalpy of combustion. On the other hand, some figures, though relatively few, are accurate within ±1 of the last digit quoted. In some ways we all inevitably fall victim to informal conventions (tradition!) about how many figures to quote for any particular property, regardless of the accuracy of individual values of that property.

In any event, we reiterate that the general intention is for the uncertainty to be between 1 and 9 in the final digit, but we know that that intention is sometimes compromised in the tables, usually for a good reason. The final piece of advice must be, if knowing the absolute accuracy really matters, consult - as a first step - the cited source (though that will not necessarily solve your problem).

TABLE 1: SIMPLE PHYSICAL PROPERTIES

(a) RELATIVE MOLECULAR MASS

The values given for relative molecular mass (molecular weight) MW are based on the 1983 IUPAC atomic weight recommendations [4]. Atomic weights taken from this source for the CHONS elements are reproduced, together with their uncertainties, in Table 1(a).

Each pure species molecular weight was first calculated as a complete summation of atomic weights over all constituent atoms of the molecule. The values listed are obtained from these by rounding at the third decimal place for species containing carbon and/or sulphur, and at the fourth decimal place for others.

The molecular weight of dry air, also rounded at the fourth decimal place, is based on the composition given in Table 1(b). This composition is collated from the work of Jones [5] and of Giacomo [6]. Note that it is the molar composition; most sources, including ISO 2533 [7], give the volumetric composition which, although only marginally different, is not strictly appropriate for direct calculation of mean molecular weight. A more important consideration, perhaps (in practical terms), is the known variability of the concentration of carbon dioxide in the atmosphere. The concentration quoted may be considered as a minimum-appropriate to the overall outside atmosphere, but substantial variations may be observed from place to place and, most particularly, in a laboratory environment. It is usual to assume that any carbon dioxide present in excess of the figure quoted displaces an equivalent amount of oxygen from the atmosphere; thus if a local concentration X of carbon dioxide is known, then the mean molecular weight M may be recalculated as

$$M = 28.9625 + 12.011\,(X - 0.00033) \qquad \text{.. (1.1)}$$

(b) NORMAL (ATMOSPHERIC) MELTING AND BOILING TEMPERATURES

Neither the melting point nor the boiling point of a substance can properly be thought of as a fundamental descriptor of the fluid phase which would normally be used in recipes for the calculation of mixture properties. Nevertheless it seems worthwhile to list these commonly observed characteristic properties.

The melting points given are, in general, actually the freezing points in air at a total pressure of 1 standard atmosphere (101.325 kPa = 1.01325 bar). An interesting exception to this is for cyclohexane; this has been shown to be a rare case for which the solubility of air in the liquid is sufficiently great to cause significant error (~0.2 K). The value given is therefore one found for air-free cyclohexane [141].

Other exceptions are for the very low ($<$ 100 K) freezing fluids, compounds which sublime at atmospheric pressure, and a few others which seem to lack a well-documented normal melting point. For all of these the triple point temperatures are given. Triple point temperatures are usually well within 0.1 K of the normal melting temperatures. Where available the triple point pressure is also given.

Both melting and boiling point temperatures are generally given on the 1968 International Practical Temperature Scale (IPTS-68) [121], as is used by all modern preferred sources. The relatively few values taken from source literature pre-dating 1968 have not been subjected to any correction; they are quoted as given, and will thus be in accordance with IPTS-48. In the range 100–450 K the difference between the two scales is everywhere less than 0.04 K.

Temperatures of fixed (defining) points or secondary reference points on IPTS-68 are quoted to 3 decimal places. All others (except for helium) are quoted to no more than 2 decimal places, though a few are believed to be better known than ±0.01 K. A variety of source literature has been used, but the TRC tabulations [145] represent the most useful general source.

There is one final, fairly topical, point which is worth mentioning in an attempt to disarm any possible confusion. This is to emphasise that the boiling temperatures given in Table 1 are all normal atmospheric boiling temperatures. That is, they refer to a boiling pressure of 1.01325 bar, not to the new thermodynamic standard state pressure, recommended by IUPAC and CODATA [8] of 1 bar. Boiling temperatures referring to a pressure of 1 bar have been termed "baric" boiling temperatures [9], but it is not yet clear if this terminology will be generally adopted; nor is it clear whether the baric boiling point will eventually supplant the atmospheric boiling point in general usage. The difference between the two is not always insignificant; for example, for water the baric boiling temperature (on IPTS-68) is 372.776 K compared, of course, with the atmospheric boiling temperature of 373.150 K. (An interesting side issue here is that the absolute thermodynamic temperature of the atmospheric boiling point is 373.125 K (i.e. 99.975°C, not 100 exactly) [9 10].)

In principle the same considerations apply to melting points. Here, however, the difference between the baric and atmospheric melting temperatures is invariably negligible at the precision level used in Table 1.

(c) THE GAS CONSTANT

The current recommended value of the gas constant R is [11]

$$R = 8.31441 \pm 0.00026 \text{ J mol}^{-1} \text{ K}^{-1} \quad .. (1.2)$$

It is expected that this value will shortly be revised to 8.31448 J mol^{-1} K^{-1}. Although use of this latter value is fairly widespread, it has not yet been formally adopted by the Commission on Data for Science and Technology (CODATA) or the International Union of Pure and Applied Chemistry (IUPAC)*. Given the latter value, the ideal gas molar volume V°_{mol} at a pressure of 1.01325 bar is

0.0224140 m^3 at 273.15 K,
0.0236449 m^3 at 288.15 K, and
0.0244655 m^3 at 298.15 K.

---

* Note added: More recent information is that the value most likely to be adopted by CODATA and IUPAC is now 8.31451 J mol^{-1} K^{-1}.

TABLE 2: CRITICAL PROPERTIES

(a) CRITICAL TEMPERATURE, PRESSURE AND DENSITY

The parameters of the gas-liquid critical point are fundamental requirements of almost all corresponding-states treatments of fluid-phase thermodynamics. Experimental observations of the critical point almost invariably document the critical temperature TC and critical pressure PC (the most commonly used reduction parameters in corresponding-states theory), less often the critical density DC or critical molar volume VC.

Here TC, PC and DC are taken as the three primary observed values for which source literature is cited. From these are derived the critical molar volume, given by

$$VC = MW/DC \qquad .. (2.1)$$

and the critical compressibility factor ZC, given by

$$ZC = MW.PC/R.TC.DC \qquad .. (2.2)$$

where R is the gas constant. Thus, for each species listed in Table 2 all five of the parameters of the critical point are internally consistent (though of course VC and ZC are rounded at an appropriate number of significant figures). ZC is sometimes used as a third reduction parameter in "extended" corresponding-states treatments of thermodynamics [12], and VC is likewise used in corresponding-states treatments of transport properties (viscosity and thermal conductivity) [13].

(b) THE ACENTRIC FACTOR AND RIEDEL PARAMETER

A more commonly used third parameter in corresponding-states thermodynamic formulations and correlations is the Pitzer acentric factor W. This is defined by

$$W = -\log(PS/PC)_{T=0.7TC} - 1 \qquad .. (2.3)$$

where PS is the saturation vapour pressure at temperature T. This seemingly strange definition was devised semi-empirically [14] as a means of assuring (a) that the crucial role of vapour pressure in determining the extent of deviation from 2-parameter "conformality" for any particular species is recognised, and (b) that simple spherical molecules, most particularly argon, which are described well by 2-parameter corresponding-states, have a near-zero third parameter. More complex and/or non-spherical (acentric) species have positive acentric factors (except for the quantum gases - hydrogen, helium, neon - which have negative values) of a magnitude which generally increases with molecular complexity.

The major sources of values for TC, PC and DC are TRC tables [145] for hydrocarbons and an NPL compilation [132] for non-hydrocarbons, although for some species other, more specific, sources have been chosen. For W, the NPL compilation is again the almost invariable source for non-hydrocarbons, and consistency with the selected TC and PC, in terms of which W is defined, is thereby assured. For hydrocarbons the usual source is a compilation published some years ago by Passut and Danner [133] and based on the then-current TRC preferred values of TC and PC; in principle, as has been emphasised by Chappelear [15], values of W should be revised whenever the corresponding TC and/or PC are revised. We have, however, retained the original acentric factors (though quoting to four decimal places is both optimistic and generally unnecessary) on the rather tenuous ground that the TRC TC and PC values have generally changed only marginally, if at all, in the period since Passut and Danner's work. For most species, the second decimal place is the last digit at which one would expect to find general agreement between independently derived values of W; correspondingly, this is probably the last digit which might be expected to exert significant influence on the derived value of a single-phase fluid property.

Yet another "third parameter" sometimes used in corresponding-states type correlations is the Riedel Parameter A. This may be calculated from the expression [137]

$$A = 0.9076 \left[1 + \left\{(TB/TC).\ln PC \,/\, \left\{1 - (TB/TC)\right\}\right\}\right] \qquad ..(2.4)$$

where TB is the normal atmospheric boiling temperature (in absolute units) and PC is in atm (not bar). Values of A may easily be derived from the data given in Tables 1 and 2, but are not listed in Table 2 because of space limitations. A simpler calculational method is to use the relationship

$$A = 4.93W + 5.808 \qquad ..(2.5)$$

A useful collection of values of A has been given by Jaeschke [16], although these do not conform exactly with either of the above two equations.

TABLE 3: STANDARD VOLUMETRIC PROPERTIES

(a) REFERENCE CONDITIONS

Two "basis state" conditions are of usual interest to the European gas industries for volumetric gas phase measurements, namely 0°C (273.15 K)/ 1.01325 bar, and 15°C (288.15 K)/1.01325 bar. These are sometimes referred to as the "normal" and "standard" state conditions respectively, but this terminology seems somewhat confusing and is best avoided (or at least made clear in the context of use). Each is "standard" in the sense that it appears in the relevant national regulatory documents for at least one European country; yet neither is "standard" in the sense of being the base condition to which thermochemists and others most often refer relevant quantities [17], namely 25°C (298.15 K)/1.01325 bar (or, more recently, 1 bar). In any event, the quantities considered in this section refer to the two conditions given above, and no others.

(b) RELATIVE DENSITY (SPECIFIC GRAVITY) AND DENSITY

The ideal relative density RD° listed for each species in Table 3 is calculated simply as

$$RD^\circ = MW/MW(air) \qquad .. (3.1)$$

As used in this document the term ideal relative density is actually defined as the ratio of the density of the sample, considered as an ideal gas, to that of air, also considered as an ideal gas at the same temperature and pressure. With this definition, the ideal relative density becomes simply equal to the ratio of the molecular weight of the sample to the molecular weight of dry air (28.9625) as in eqn.(3.1).

Occasionally, however [18 19], ideal relative density is defined differently, as the ratio of the density of the sample, considered as an ideal gas, to that of <u>real</u> air at the same temperature and pressure. In this definition the value is equal to the ratio of molecular weights multiplied by the compressibility factor of air, through which value it is a function of temperature and pressure. That definition is <u>not</u> used here.

In any event, whichever of the above definitions is used, the real-gas relative densities at the two base states are given by

$$RD(0) = MW/MW(air) \times Z(air,0)/Z(0) \qquad .. (3.2)$$

$$RD(15) = MW/MW(air) \times Z(air,15)/Z(15) \qquad .. (3.3)$$

where all compressibility factor values refer to a pressure of 1.01325 bar. Values for RD(0) and RD(15) are given in Table 3. Note that many of these values are for the hypothetical gas, through the use of a hypothetical gas-phase compressibility factor of a species not actually gaseous at the given base conditions.

Not listed, for space reasons, in Table 3 are the corresponding ideal and real actual mass densities. These are given (in kg m^{-3}), using obvious notation, by

$$D^\circ(0) = MW.P/R.T1 \qquad .. (3.4)$$

$$D^\circ(15) = MW.P/R.T2 \qquad .. (3.5)$$

$$D(0) = D^{\circ}(0)/Z(0) \quad .. (3.6)$$

$$D(15) = D^{\circ}(15)/Z(15) \quad .. (3.7)$$

where T1 = 273.15 K, T2 = 288.15 K and P = 101.325 kPa. Note again that such definitions do not automatically prevent one from calculating hypothetical - spurious - gas-phase densities for species which are actually liquid at the relevant condition.

(c) COMPRESSIBILITY FACTORS AND SECOND VIRIAL COEFFICIENTS

In order to obtain values for the real-gas densities and relative densities for individual species and, by appropriate combination of these [3 19], for specified mixtures, it is obviously necessary to know the compressibility factor for each (possibly hypothetical) gas at each relevant condition. They are also needed for the calculation of calorific value from the ISO 6976 recipe [3] (which is based on an old IGT method [20]). In this sense they are the most basic properties listed in Table 3.

Wherever possible, most obviously for the "permanent" gases, it is of course preferable to use compressibility factors taken directly from experiment, or at least from the fitting of high-quality PVT-data to a good interpolative equation of state. The values given in Table 3 have generally been taken from secondary compilations, notably that of Armstrong and Jobe [103], which satisfy this criterion.

However, for species which are not actually gaseous at the conditions of interest a different approach is needed. In each such case a hypothetical value of Z has been calculated as the solution of the truncated virial equation

$$P.V_{mol}/R.T = Z = 1 + B.P/Z.R.T \quad .. (3.8)$$

where B is the second virial coefficient and other terms have their obvious significance. B is a function of T but not of P. Values of B can be obtained either from PVT-data taken at pressures below the saturation vapour pressure, or from some form of generalised correlation.

For most hydrocarbons in this "non-gaseous" category the latter approach was adopted. From the several correlations available [21 135 146], we in fact chose a simplified version of the oldest corresponding-states type correlation, the Pitzer-Curl equation [135]. The reason for this choice, and for the way in which we chose to simplify it was the observation that, of all the various means of calculating Z tested, this gave marginally the best values for those similar species for which more direct values of Z are otherwise available.

The Pitzer-Curl expression for B is

$$
\begin{aligned}
B.PC/R.TC = {} & (0.1445 + 0.073W) - (0.330 - 0.46W)/T_r \\
& - (0.1385 + 0.50W)/T_r^{2} - (0.0121 + 0.097W)/T_r^{3} \\
& - 0.0073W/T_r^{8} \qquad .. (3.9)
\end{aligned}
$$

where $T_r = T/TC$, T being either 273.15 K or 288.15 K for the present application. Values for TC, PC and W are given in Table 2. For the calculation of Z values from Pitzer-Curl B values so obtained, a linearised approximation of eqn.(3.8) was used, i.e. the second term on the right hand side was taken simply as BP/RT. (In fact, if the full (un-linearised) expression (3.8) is used, a large negative value of B is reached for hydrocarbons above C_7, beyond which there is <u>no</u> real solution for Z.)

The Pitzer-Curl correlation is, in principle, only applicable to non-polar hydrocarbons. Thus for non-hydrocarbons other methods of estimating B should be found. Our main resort in these cases was to rough interpolation or extrapolation of second virial coefficients listed in ref.110.

Values of Z (at 273.15 K/1.01325 bar and 288.15 K/1.01325 bar) and B (for reasons of space at 288.15 K only) are listed in Table 3 for all species.

TABLE 4: ENTHALPIES OF FORMATION AND COMBUSTION

(a) STANDARD ENTHALPIES OF FORMATION AND COMBUSTION

The two *fundamental* quantities given in Table 4 are (1) the standard molar enthalpy of formation of the species from its elements at 25°C $\Delta_f H^\circ(25)$, and (2) the standard molar enthalpy of combustion of the species at 25°C $\Delta_c H^\circ(25)$, in accordance with the generalised combustion equation

$$C_aH_bO_cN_dS_e\ (g) + (a + b/4 - c/2 + e)\ O_2\ (g)$$

$$= a\ CO_2\ (g) + b/2\ H_2O\ (\ell) + d/2\ N_2\ (g) + e\ SO_2\ (g) \qquad .. (4.1)$$

The thermodynamic (or thermochemical) standard state of a pure gas is that of the hypothetical ideal gas at a pressure of 1 bar (new IUPAC standard state) or 1.01325 bar (old IUPAC standard state) [17]. In fact the standard enthalpies of formation and combustion are independent of pressure [9] (because of ideality), and are equal to the real-gas enthalpies at zero pressure and the same temperature.

For both $\Delta_f H^\circ(25)$ and $\Delta_c H^\circ(25)$, the values in Table 4 are consequently always for the species in the hypothetical ideal gas state, even when the thermodynamically stable state for a species is a condensed phase. Additionally all the other reactants and products in formation and combustion reactions are taken to be in the ideal-gas state, except for carbon (as graphite) in formation reactions, and water (as liquid) as a product in combustion reactions (but still in the gas phase elsewhere).

The two quantities $\Delta_f H^\circ(25)$ and $\Delta_c H^\circ(25)$ are unambiguously related to each other for each species by the expressions (with the temperature assignment omitted for clarity) -

$$\Delta_f H^\circ = -\Delta_c H^\circ + a.\Delta_f H^\circ(CO_2,g) + b/2.\Delta_f H^\circ(H_2O,\ell) + e.\Delta_f H^\circ(SO_2,g) \qquad .. (4.2)$$

$$= -\Delta_c H^\circ + a.\Delta_f H^\circ(CO_2,g) + b/2.\Delta_c H^\circ(H_2,g) + e.\Delta_f H^\circ(SO_2,g) \qquad .. (4.3)$$

Since $\Delta_c H^\circ$ is always negative (or zero) and $\Delta_f H^\circ$ is most often negative, a great deal of care with signs is necessary when handling equations of this sort.

In Table 4 all of the values given for $\Delta_f H^\circ(25)$ and $\Delta_c H^\circ(25)$ are consistent with each other in accordance with the above equations, using the CODATA recommended values [109] of $\Delta_f H^\circ(CO_2,g)$ (-393.51 kJ mol^{-1}), $\Delta_c H^\circ(H_2,g)$ (-285.83) and $\Delta_f H^\circ(SO_2,g)$ (-296.81). The values given have been taken from a variety of sources, most notably from the TRC compilation [145] and from the recent $\Delta_c H^\circ$ re-evaluations by Garvin *et al* [114]. For cases where self-consistent pairs of values could not be found in the literature, a favoured value (either $\Delta_f H^\circ$ or $\Delta_c H^\circ$) was taken and the "conjugate" value calculated from it by the present author [101] in accordance with the above equations.

The remaining standard enthalpies of combustion $\Delta_c H^\circ(15)$ given in Table 4 are related to the corresponding values of $\Delta_c H^\circ(25)$ in accordance with the expressions

$$\Delta_c H^\circ(15) = \Delta_c H^\circ(25) + \sum_i \nu_i \left[H_i^\circ(25) - H_i^\circ(15)\right] \quad .. (4.4)$$

$$= \Delta_c H^\circ(25) + \sum_i \int_{15}^{25} \nu_i C_{p,i}^\circ \cdot dt \quad .. (4.5)$$

where H_i° is the ideal-gas enthalpy and $C_{p,i}^\circ$ is the ideal-gas heat capacity at constant pressure of species i (except for product water which is taken as the liquid). The summation is taken over all species i in the combustion reaction, eqn. (4.1); ν_i is the stoichiometric coefficient of species i, being taken as positive for reactants (unity for the "object" species) and negative for products. For brevity we designate the whole of the second term on the the right-hand side of eqn. (4.4) and (4.5) as ΔH°.

ΔH° is always very small in comparison with $\Delta_c H^\circ$, to which it can clearly be considered as a correction term. For the purposes of Table 4, values of $\Delta_c H^\circ(15)$ have either been taken directly from the work of Garvin <u>et al</u> [114], or have been derived, via ΔH°, by the present author [120]. Only brief outlines of such derivations are given here.

For a few gases ΔH° was calculated using $H^\circ(25) - H^\circ(15)$ data given in Armstrong and Jobe [103] for "auxiliary" species such as O_2, H_2, CO, CO_2 and H_2O. For most (but not all) other cases calculations are able to be made using the polynomial $C_p^\circ(T)$ fits given by Passut and Danner [22]. However, as a preferred alternative we used for all remaining cases a computer program which can calculate the ideal-gas enthalpy at any temperature in the range 100–1000 K (at least), for any species of present interest, by use of a polynomial expression generally of the Wilhoit-Harmens form [23 24], but incorporating improvements which have not yet been publicly documented. Checks against the Garvin <u>et al</u> data [114], Armstrong and Jobe data [103], and values of ΔH° calculated using Passut and Danner polynomials [22] did not reveal any significant discrepancies.

(b) REAL-GAS ENTHALPIES OF COMBUSTION

The real-gas enthalpy of combustion of any species is related to the ideal-gas (standard) enthalpy of combustion at the same temperature T by

$$\Delta_c H(T) = \Delta_c H^\circ(T) + \sum_i \nu_i \left[H_i^\circ(T) - H_i(T,P^\circ)\right] \quad .. (4.6)$$

$$= \Delta_c H^\circ(T) + \sum_i \nu_i \left[H_i(T,0) - H_i(T,P^\circ)\right] \quad .. (4.7)$$

where $H_i(T,P)$ is the real-gas enthalpy of species i at temperature T and pressure P ; P° (=1.01325 bar) is the pressure of the real-gas reference state. The summation is taken over all species i in the combustion reaction eqn. (4.1), except for (liquid) water. As before, the stoichiometric coefficients ν_i are taken to be positive for reactants, negative for products. For brevity we designate the whole of the second term on the right-hand side side of eqn. (4.6) and (4.7) as δH.

As was the case for ΔH°, values of δH are very small (but non-negligible) in comparison with $\Delta_c H^\circ$. Values of δH have been derived for $t = 0, 15$ and 25°C at the U.S. National Bureau of Standards (NBS) [103 114 125] for several of those species of interest here which are actually gaseous at the relevant conditions. Values of $\Delta_c H(T)$ derived from $\Delta_c H^\circ(T)$ using these values of $\delta H(T)$ are given in Table 4. For species *not* considered in the NBS documents, values of δH have been derived by the present author by use of the LRS equation of state [25]. This relatively new cubic equation of state is a development of the popular Redlich-Kwong-Soave equation [26], which itself is quite reliable for the calculation of gas-phase enthalpies. The LRS equation of state characterises each molecular species by means of a pair of empirically determined constants (in addition to TC and PC) which are obtained by optimising the fit to as much of the complete vapour pressure curve, from the triple point to the critical point, as is reliably available. Not all of these characteristic constants have yet been reported in the open literature. The LRS equation of state is similar in many respects to that devised independently by Mathias [27].

As a final reminder that one of the trickiest aspects of the manipulation of enthalpic data, such as that contained in Table 4 and/or mentioned above, is the matter of signs, note that *all* data columns in Table 4 carry a *negative* heading.

TABLE 5: CALORIFIC VALUES

(a) VOLUME-BASED GROSS CALORIFIC VALUES

The volume-based calorific value (C.V.) of a fuel gas is defined as the amount of heat released by complete combustion in air, at constant (specified) pressure, of a volumetrically-defined amount of gas, with the products of combustion being returned to the same (specified) temperature as that of the reactants prior to combustion.

If all of the water of combustion is condensed to the liquid phase (a practical impossibility), then the C.V. so defined is the gross, superior, upper, higher or total calorific value; if all of the water of combustion remains in the vapour phase, then the C.V. is the net, inferior or lower calorific value. All C.Vs listed in this compilation are gross. (An interesting oddity resulting from the definition of gross C.V. is that the contribution of any gas-phase water (humidity) to the gross C.V. of a gas mixture is non-zero, i.e. water vapour has a small but non-negligible gross calorific value derivable from its enthalpy of vaporisation (latent heat) at an appropriate temperature, despite being incombustible [28].)

The calorific value of a gaseous fuel can be referred to any one of a remarkable variety of so-called "standard" (or base) conditions, each of which has two determinants, viz.

(1) the temperature (and pressure) at which combustion is deemed to take place, and

(2) the temperature (and pressure) at which the gaseous fuel is deemed to be metered.

There is really no logical reason why the temperatures referred to in (1) and (2) have to be the same, and there are 3 fairly obvious choices for each, namely 0°C (273.15 K), 15°C (288.15 K) and 25°C (298.15 K). Fortunately only a single pressure condition (1.01325 bar) is currently in use with (metric) calorific values - although 1 bar appears to be a distinct future possibility.

Since, however, the metric units of calorific value are always the same irrespective of the pair of conditions chosen for reference, considerable confusion can be caused to the uninitiated user of C.V. tabulations. The current edition of ISO 6976 [3], for example, quotes values (in $\mathrm{kJ\ m^{-3}}$) for 4 of these "metric" temperature pairings, namely 25°C (combustion)/0°C (metering), 15°/0°, 0°/0° and 15°/15° (it also quotes the old Imperial 60°F condition, but that is of no relevance here).

Fortunately, not all of the 9 possible combinations are actually in use. Which condition is used by the gas industry of any particular country is in fact determined, of course, by the national metrological statutes of that country. For instance, the U.K. uses 15/15, much of continental Europe uses 25/0 and Japan uses 0/0.

In any event, largely for space reasons, Table 5 of this compilation includes values for just 3 conditions, namely 25/0, 15/0 and 15/15. For each of the 3 conditions, calorific values are given for each species in both the (hypothetical) ideal gas state (CV°) and, if the species actually is gaseous at the relevant reference conditions, for the real-gas state (CV). The quantities CV° are those most often given in tabulations whose objective is to facilitate the calculation of real-gas mixture calorific values from known composition, often by a recipe [3 19 20] which, while sufficiently accurate, is not thermodynamically rigorous [28 103].

The values given in Table 5 have been derived entirely from values given in Tables 3 and 4 in accordance with the following equations -

$$CV°(25/0) = -\Delta_c H°(25) \times P/R.T_1 \quad .. (5.1)$$

$$CV\ (25/0) = -\Delta_c H(25) \times P/Z(T_1).R.T_1 \quad .. (5.2)$$

$$CV°(15/0) = -\Delta_c H°(15) \times P/R.T_1 \quad .. (5.3)$$

$$CV\ (15/0) = -\Delta_c H(15) \times P/Z(T_1).R.T_1 \quad .. (5.4)$$

$$CV°(15/15) = -\Delta_c H°(15) \times P/R.T_2 \quad .. (5.5)$$

$$CV\ (15/15) = -\Delta_c H(15) \times P/Z(T_2).R.T_2 \quad .. (5.6)$$

where P = 101.325 kPa, T1 = 273.15 K, T2 = 288.15 K. Used with R = 8.31448 J mol^{-1} K^{-1}, these expressions convert $\Delta_c H$ in kJ mol^{-1} to CV in MJ m^{-3}.

Other data from Tables 3 and 4 allow the derivation by similar means for at least some of the calorific values for the conditions denoted by 25/15, 0/15, and 0/0 which for space reasons are excluded from Table 5.

The important point about the values given in Table 5 is that for each distinct chemical species the six calorific values listed form an internally consistent set, in the senses that

(1) the "enthalpic" part of the C.V. is always based directly on, or by traceable derivation from, the single selected value of $\Delta_c H°(25)$ given in Table 4, and

(2) the "volumetric" part of the real-gas C.V. is always based on a value of the compressibility factor Z which is derived either from direct experiment, or from an established functional form applicable at each temperature of interest (e.g. the Pitzer-Curl equation [135]).

In order to avoid any possible confusion it should be stressed again that all of the values listed are gas-phase (hypothetical or real) calorific values. No liquid phase calorific values are given.

(b) VOLUME-BASED NET CALORIFIC VALUES

Although net calorific values are not listed in this compilation they may easily be derived from the corresponding gross calorific values by the following expressions

$$CV°(net) = CV°(gross) \times \left[(\Delta_c H°(T) - f.\Delta_v H°(T))/\Delta_c H°(T)\right] \quad .. (5.7)$$

$$CV(net) = CV(gross) \times \left[(\Delta_c H(T) - f.\Delta_v H(T))/\Delta_c H(T)\right] \quad .. (5.8)$$

where $\Delta_v H^\circ(T)$ is the (standard) enthalpy of vaporisation of liquid water to the ideal gas state at the "combustion" reference temperature T, $\Delta_v H(T)$ is the enthalpy of vaporisation of liquid water to the real-gas state (latent heat) at the same temperature, and f (= -b/2) is the (negative) stoichiometric coefficient of the product water in the combustion equation (see previous section). Note that $\Delta_c H$ is a negative quantity, $\Delta_v H$ positive.

(c) MASS-BASED GROSS CALORIFIC VALUES

It is sometimes useful to have available the calorific value per unit mass, rather than volume, of a fluid. For gaseous substances, these may be easily derived by dividing (-) the appropriate molar enthalpy of combustion from Table 4 by the molar mass (numerically equal to the molecular weight, but attributed units of kg mol^{-1}) from Table 1. Clearly, several such quantities could be listed; we give just one, namely the real-gas gross calorific value Q per unit mass (MJ kg^{-1}), at 298.15 K (25°C) and 1.01325 bar, given by

$$Q = -\Delta_c H(25)/MW \qquad .. (5.9)$$

Mass-based calorific values are, in principle, somewhat simpler than volume-based C.Vs because there is no potential confusion about the reference state for volume measurement. Unfortunately it is much easier, on a routine basis, to meter gaseous fuels by volume than by mass. Nevertheless for some applications, for example in the determination of the gas-phase energy contained in a bulk liquefied natural gas cargo, mass-based C.Vs are undoubtedly of greater direct utility.

TABLE 6: FLAMMABILITY DATA

(a) FLAMMABILITY LIMITS IN AIR

No fuel-gas or gas mixture will burn when mixed homogeneously with air unless the relative amount of fuel to total mixture is within certain limits which are characteristic of the fuel. The lower limit of flammability LL is defined as the smallest proportion of fuel-gas to total fuel-air mixture in which combustion, once initiated, will propagate throughout the mixture; similarly the upper limit of flammability LU is the greatest proportion of fuel-gas to total fuel-air mixture in which combustion will propagate.

Although the flammability limits are important characteristic properties of a pure gas, no successful "first-principles" derivation (as opposed to a correlation) of any has ever been made. Thus the limits should be determined experimentally. For various reasons [29], it is not easy to determine the "true" flammability limits. Consequently if there is any experimental doubt about a precise limit, then that which implies the widest range of flammability in air is usually quoted for reasons of safety-consciousness. That view is generally adopted here. An exception to this, however, is the interim (at least) exclusion of some recent data [30] which suggest rather wider limits for methane (4.4 to 16.5% by volume) and ethylene than have hitherto been reported and supported independently. The new values have been excluded not only for this reason, but also because the apparatus used is of a form not previously used in such studies, so that there remains a possibility that the values are somewhat artefactual. In addition the criterion of flammability adopted is unusual. It should be appreciated that close to the limits, particularly the upper, it may often be rather difficult to inflame the gas.

Table 6 gives values for both the upper and lower flammability limits as percent by volume of the total gas plus nominally dry air mixture. Several sources have been used, mostly notably the Nabert-Schön [130] and ESDU [112] compilations. All values are intended to refer to a temperature of 25°C and to a total pressure of 1 atm., but some have actually been determined at other conditions.

Minor variations of temperature around ambient have no significant effect upon flammability limits, but for large temperature variations the consequences may be important. The general effect is for an increase in temperature to widen the limits of flammability. The depression of the lower limit and elevation of the upper both appear to be roughly proportional to the increase in temperature. For the alkanes and alkenes the dependence on temperature is in accord with the modified Burgess-Wheeler law, viz.

$$L(t) = L(25)\left[1 \pm 7.2\ 10^{-4}\ (t-25)\right] \qquad ..\ (6.1)$$

where $L(t)$ is the flammability limit at a Celsius temperature t and $L(25)$ is the limit for $t = 25°C$. The positive sign is used for LU and the negative sign for LL [152].

Likewise the normal variations of atmospheric pressure do not appreciably affect the flammability limits. Reduction of pressure significantly below atmospheric brings about an elevation of the lower limit and depression of the upper limit, until at a suitably low pressure the limits coincide; below this limit no flame can propagate. The limiting pressure is about 100 torr ($\sim 1.3\ 10^4$ Pa) for methane and about 50 torr for a gas mixture comprising ~80% methane and ~20% ethane [29].

Large increases in pressure above ambient also have significant effects, but there is no clear general trend. The extent of the effect, however, can be very marked, e.g. the upper limit of flammability for methane rises fairly linearly from 15% at 1 atm to about 35% at 75 atm, although there is little effect on the lower limit[29].

The effect on flammability limits of atmospheric humidity is thought to be simply that of replacement by water vapour of oxygen that would otherwise be available to support combustion. Since there is always sufficient oxygen available at the lower limit, no noticeable effect upon this limit occurs. The upper limit, however, will of necessity be lowered slightly if the air for combustion is damp. For methane the lowering of the upper limit brought about by the replacement of dry air by saturated air is about ½%[29].

(b) MINIMUM AUTOIGNITION TEMPERATURE

Table 6 also lists for each species the lowest temperature for which spontaneous ignition may occur in the gas or vapour phase - at any fuel/air ratio. This is called the minimum autoignition temperature. It is a purely empirical property. Most of the values listed are taken from the Stull[142] and Nabert-Schön[130] compilations. One important exception is the value for methane[138], which at 874 K (601°C) is some 60 K higher than that given in most compilations. It appears, however, that the lower values (around 540°C) are <u>not</u> based upon experiment; the value quoted here[138] is the lowest experimentally observed value.

CONCLUDING REMARKS

No compilation of this sort is ever as complete as either the authors or the users would wish; there is always "one more species" which should not have been excluded, and we are well aware of several more properties which could usefully have been included. The only defence is to assert that clearly there must be a quite restrictive limitation if the objective is to give widespread currency to a freely available set of data in a "hard-copy" format.

It should almost go without saying that the real solution, particularly for the compiler who is much concerned with the problem of maintaining currency without the necessity for constant reprinting, is the computerised databank. But there is apparently much peace of mind to be had, even for the confirmed computer-user, by ownership of a "hard-copy" set of basic data, especially if these are "recommended" or "approved" by an identifiable authority such as, in this instance, the G.E.R.G. Thermodynamics Committee hopes to find itself considered.

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TABLE 1(a)

ATOMIC WEIGHTS OF SELECTED ELEMENTS

Element	Atomic Weight	Uncertainty (in last digit)
C	12.011	1
H	1.00794	7
O	15.9994	3
N	14.0067	1
S	32.066	6

TABLE 1(b)

MOLAR COMPOSITION OF DRY AIR

Species	Mole Percent
Nitrogen	78.102
Oxygen	20.946
Argon	0.916
Carbon Dioxide	0.033
Neon	0.00182
Helium	0.00052
Methane	0.00015
Krypton	0.00011
Hydrogen	0.00005
Nitrous Oxide	0.00003
Carbon Monoxide	0.00002
Xenon	0.00001

FOOTNOTES FOR TABLES

a	Molar composition of dry air given in Table 1(b).
b	All properties given for normal hydrogen.
c	All properties given for helium-4.
h	Calculated value for the hypothetical gas.
ℓ	Species liquid at this condition.
n	Species non-flammable.
s	Sublimation point.
t	Triple point.
u	Lambda point.

TABLE 1

SIMPLE PHYSICAL PROPERTIES

		Note	ATOMIC CONSTITUTION C	H	O	N	S	X	RELATIVE MOLECULAR MASS	ATMOSPHERIC MELTING TEMPERATURE / K	Note	Reference	ATMOSPHERIC BOILING TEMPERATURE / K	Note	Reference	TRIPLE POINT PRESSURE / Pa	Note	Reference
1	METHANE		1	4					16.043	90.685	t	BED	111.66		BED	11696		PCF
2	ETHANE		2	6					30.070	90.35	t	BED	184.55		TRC.85	1.2		STS
3	PROPANE		3	8					44.097	85.52	t	BED	231.07		TRC.85	0.0003		CAR
4	n-BUTANE		4	10					58.123	134.79		TRC.85	272.64		TRC.85			
5	2-METHYLPROPANE		4	10					58.123	113.54		TRC.85	261.36		TRC.85			
6	n-PENTANE		5	12					72.150	143.42		TRC.85	309.22		TRC.85			
7	2-METHYLBUTANE		5	12					72.150	113.25		TRC.85	300.99		TRC.85			
8	2,2-DIMETHYLPROPANE		5	12					72.150	256.58		TRC.85	282.65		TRC.85			
9	n-HEXANE		6	14					86.177	177.83		TRC.77	341.89		TRC.77			
10	2-METHYLPENTANE		6	14					86.177	119.48		TRC.65	333.41		TRC.75			
11	3-METHYLPENTANE		6	14					86.177	155.2		AWU	336.43		TRC.75			
12	2,2-DIMETHYLBUTANE		6	14					86.177	173.29		TRC.65	322.88		TRC.75			
13	2,3-DIMETHYLBUTANE		6	14					86.177	144.61		TRC.65	331.13		TRC.75			
14	n-HEPTANE		7	16					100.204	182.57		TRC.77	371.57		TRC.77			
15	n-OCTANE		8	18					114.231	216.39		TRC.77	398.82		TRC.77			
16	n-NONANE		9	20					128.258	219.66		TRC.79	423.95		TRC.79			
17	n-DECANE		10	22					142.285	243.49		TRC.79	447.27		TRC.79			
18	ETHENE		2	4					28.054	104.00		YOU	169.41		YOU			
19	PROPENE		3	6					42.081	87.91	t	TRC.81	225.43		TRC.81	0.0004		GAZ
20	1-BUTENE		4	8					56.108	87.80	t	TRC.81	266.92		TRC.81			
21	cis-2-BUTENE		4	8					56.108	134.24		TRC.65	276.87		TRC.72			
22	trans-2-BUTENE		4	8					56.108	167.60		TRC.65	274.03		TRC.72			
23	2-METHYLPROPENE		4	8					56.108	132.80		TRC.65	266.24		TRC.72			
24	1-PENTENE		5	10					70.134	107.93		TRC.81	303.11		TRC.81			
25	PROPADIENE		3	4					40.065	136.85		SWS	238.8		ZWO			
26	1,2-BUTADIENE		4	6					54.092	136.96		SWS	284.00		ZWO			
27	1,3-BUTADIENE		4	6					54.092	164.24		SWS	268.74		ZWO			

28	ETHYNE		2	2					26.038	192.60	t	STV	189.35	s	MIL	128190		STV
29	CYCLOPENTANE		5	10					70.134	179.27		TRC.68	322.40		TRC.75			
30	METHYLCYCLOPENTANE		6	12					84.161	130.72		TRC.65	344.96		ZWO			
31	ETHYLCYCLOPENTANE		7	14					98.188	134.70		TRC.65	376.62		ZWO			
32	CYCLOHEXANE		6	12					84.161	279.88		STT	353.88		TRC.75			
33	METHYLCYCLOHEXANE		7	14					98.188	146.56		TRC.65	374.08		ZWO			
34	ETHYLCYCLOHEXANE		8	16					112.215	161.83		TRC.65	404.95		ZWO			
35	BENZENE		6	6					78.114	278.68		TRC.85	353.24		TRC.85			
36	TOLUENE		7	8					92.141	178.19		TRC.85	383.78		TRC.85			
37	ETHYLBENZENE		8	10					106.167	178.20		TRC.85	409.35		TRC.85			
38	o-XYLENE		8	10					106.167	247.98		TRC.85	417.58		TRC.85			
39	METHANOL		1	4	1				32.042	175.47		WIL	337.85		WIL			
40	METHANETHIOL		1	4			1		48.109	150.18		TRC.65	279.11		ZWO			
41	HYDROGEN	b		2					2.0159	13.958	t	BED	20.397		BED	7200		GAZ
42	WATER			2	1				18.0153	273.150		BED	373.150		IPT			
43	HYDROGEN SULPHIDE			2			1		34.082	187.67	t	TRC.84	212.88		TRC.84	23180		TRC.84
44	AMMONIA			3		1			17.0305	195.48	t	STV	239.82		HAG	6077		HAG
45	HYDROGEN CYANIDE		1	1		1			27.026	259.91		SWS	298.85		SWS			
46	CARBON MONOXIDE		1		1				28.010	68.13	t	GOO	81.64		GOO	15400		GOO
47	CARBONYL SULPHIDE		1		1		1		60.076	134.34		SWS	222.92		SWS			
48	CARBON DISULPHIDE		1				2		76.143	161.26	t	STV	319.37		WSW			
49	HELIUM	c						1	4.0026	2.177	u	MCY	4.224		MCY	5035	u	MCY
50	NEON							1	20.179	24.562	t	BED	27.102		IPT	43356		STV
51	ARGON							1	39.948	83.798	t	IPT	87.295		BED	68890		BOP
52	NITROGEN					2			28.0134	63.146	t	BED	77.344		BED	12527		STV
53	OXYGEN				2				31.9988	54.361	t	IPT	90.188		IPT	147		STV
54	CARBON DIOXIDE		1		2				44.010	216.580	t	BED	194.673	s	BED	518500		TRC.84
55	SULPHUR DIOXIDE				2		1		64.065	197.68	t	TRC.84	263.13		TRC.84	1675		STV
	AIR	a							28.9625									

TABLE 2

CRITICAL PROPERTIES

		CRITICAL TEMPERATURE / K	Reference	CRITICAL PRESSURE / bar	Reference	CRITICAL DENSITY / kg m^{-3}	Reference	CRITICAL MOLAR VOLUME / cm^3 mol^{-1}	CRITICAL COMPRESSIBILITY FACTOR	ACENTRIC FACTOR	Reference
1	METHANE	190.555	MCC	45.988	MCC	164.1	MCC	97.76	0.284	0.0115	HED
2	ETHANE	305.83	TRC.84	48.80	TRC.84	203	TRC.84	148.1	0.284	0.0908	PAD
3	PROPANE	369.82	TRC.84	42.50	TRC.84	217	TRC.84	203.2	0.281	0.1454	PAD
4	n-BUTANE	425.14	KSM	37.84	KSM	228	TRC.84	254.9	0.273	0.1928	PAD
5	2-METHYLPROPANE	408.13	TRC.84	36.48	TRC.84	221	TRC.84	263.0	0.283	0.1756	PAD
6	n-PENTANE	469.69	KRA	33.64	KRA	232	KRA	311.0	0.268	0.2510	PAD
7	2-METHYLBUTANE	460.39	TRC.84	33.81	TRC.84	236	TRC.84	305.7	0.270	0.2273	PAD
8	2,2-DIMETHYLPROPANE	433.75	TRC.84	31.99	TRC.84	238	TRC.84	303.2	0.269	0.1970	PAD
9	n-HEXANE	506.4	TRC.84	30.3	TRC.84	233	TRC.84	369.9	0.266	0.2957	PAD
10	2-METHYLPENTANE	497.5	TRC.84	30.1	TRC.84	235	TRC.84	366.7	0.267	0.2791	PAD
11	3-METHYLPENTANE	504.4	TRC.84	31.2	TRC.84	235	TRC.84	366.7	0.273	0.2750	PAD
12	2,2-DIMETHYLBUTANE	488.7	TRC.84	30.8	TRC.84	240	TRC.84	359.1	0.272	0.2310	PAD
13	2,3-DIMETHYLBUTANE	499.9	TRC.84	31.3	TRC.84	241	TRC.84	357.6	0.269	0.2473	PAD
14	n-HEPTANE	539.2	TRC.84	27.4	TRC.84	232	TRC.84	431.9	0.264	0.3506	PAD
15	n-OCTANE	568.4	TRC.84	24.9	TRC.84	232	TRC.84	492.4	0.259	0.3942	PAD
16	n-NONANE	594.4	TRC.84	22.8	TRC.84	232	TRC.84	552.8	0.255	0.4437	PAD
17	n-DECANE	617.8	TRC.84	20.9	TRC.84	233	TRC.84	610.7	0.248	0.4902	PAD
18	ETHENE	282.35	TRC.84	50.42	TRC.84	214	TRC.84	131.1	0.282	0.0856	PAD
19	PROPENE	364.85	TRC.84	46.01	TRC.84	232	TRC.84	181.4	0.275	0.1477	PAD
20	1-BUTENE	419.53	TRC.84	40.23	TRC.84	234	TRC.84	239.8	0.277	0.1874	PAD
21	cis-2-BUTENE	435.58	TRC.77	42.2	TRC.77	240	TRC.77	233.8	0.272	0.2044	PAD
22	trans-2-BUTENE	428.63	TRC.77	40.5	TRC.77	236	TRC.77	237.7	0.270	0.2138	PAD
23	2-METHYLPROPENE	417.90	TRC.77	40.0	TRC.77	235	TRC.77	238.8	0.275	0.1898	PAD
24	1-PENTENE	464.78	TRC.84	35.26	TRC.84	237	TRC.84	295.9	0.270	0.2450	PAD
25	PROPADIENE	393	TRC.48	54.7	RPS	247	RPS	162	0.271	0.149	EDM
26	1,2-BUTADIENE	443.7	PAD	45.0	PAD	247	RPS	219	0.267	0.3394	PAD
27	1,3-BUTADIENE	425	TRC.48	43.3	TRC.48	245	TRC.48	221	0.271	0.1814	PAD

28	ETHYNE	308.33	TRC.67	61.39	TRC.67	231	TRC.67	112.7	0.270	0.1841	PAD
29	CYCLOPENTANE	511.61	TRC.75	45.02	TRC.75	270	TRC.75	259.8	0.275	0.1923	PAD
30	METHYLCYCLOPENTANE	532.73	TRC.67	37.84	TRC.67	264	TRC.67	318.8	0.272	0.2395	PAD
31	ETHYLCYCLOPENTANE	569.46	TRC.67	33.97	TRC.67	262	TRC.67	374.8	0.269	0.2826	PAD
32	CYCLOHEXANE	553.5	TRC.75	40.74	TRC.75	271.8	TRC.75	309.6	0.274	0.2144	PAD
33	METHYLCYCLOHEXANE	572.12	TRC.67	34.71	TRC.67	267	TRC.67	367.7	0.268	0.2333	PAD
34	ETHYLCYCLOHEXANE	609	TRC.67	30.4	TRC.67	250	TRC.67	449	0.269	0.2426	PAD
35	BENZENE	562.16	TRC.79	48.98	TRC.79	304.4	TRC.79	256.6	0.269	0.2100	PAD
36	TOLUENE	591.80	TRC.79	41.06	TRC.79	291.3	TRC.79	316.3	0.264	0.2566	PAD
37	ETHYLBENZENE	617.20	TRC.79	36.06	TRC.79	283.5	TRC.79	374.5	0.263	0.3011	PAD
38	o-XYLENE	630.33	TRC.79	37.34	TRC.79	288	TRC.79	368.6	0.263	0.3136	PAD
39	METHANOL	512.64	NPL	80.92	NPL	272	NPL	117.8	0.224	0.556	NPL
40	METHANETHIOL	470.0	NPL	72.3	NPL	332	NPL	144.9	0.268	0.153	NPL
41	HYDROGEN	33.2	NPL	12.97	NPL	31	NPL	65.0	0.306	-0.218	NPL
42	WATER	647.14	LEV	220.64	LEV	322	LEV	55.9	0.229	0.328	NPL
43	HYDROGEN SULPHIDE	373.2	NPL	89.4	NPL	346	NPL	98.5	0.284	0.109	NPL
44	AMMONIA	405.5	NPL	113.5	NPL	235	NPL	72.5	0.244	0.250	NPL
45	HYDROGEN CYANIDE	456.7	NPL	53.9	NPL	195	NPL	138.6	0.197	0.388	NPL
46	CARBON MONOXIDE	132.85	GOO	34.94	GOO	304	GOO	92.2	0.291	0.053	NPL
47	CARBONYL SULPHIDE	378.8	ROB	63.49	ROB	445	ROB	135.1	0.272	0.096	ROB
48	CARBON DISULPHIDE	552	NPL	79.0	NPL	440	NPL	173.1	0.298	0.109	NPL
49	HELIUM	5.19	NPL	2.27	NPL	70	NPL	57.2	0.301	-0.365	NPL
50	NEON	44.40	NPL	27.6	NPL	484	NPL	41.7	0.312	-0.029	NPL
51	ARGON	150.65	WIT	48.66	WIT	529.1	WIT	75.5	0.293	0.001	NPL
52	NITROGEN	126.2	NPL	33.9	NPL	313	NPL	89.5	0.289	0.039	NPL
53	OXYGEN	154.58	NPL	50.43	NPL	436	NPL	73.4	0.288	0.025	NPL
54	CARBON DIOXIDE	304.20	ANG	73.86	ANG	468	ANG	94.0	0.275	0.239	NPL
55	SULPHUR DIOXIDE	430.8	NPL	78.84	ANG	525	NPL	122.0	0.269	0.256	NPL
	AIR	132.55	NPL	37.69	NPL	313	NPL	92.5	0.316		

TABLE 3

STANDARD VOLUMETRIC PROPERTIES

		COMPRESSIBILITY FACTOR @ 0°C, 1.01325 bar	Note	Reference	COMPRESSIBILITY FACTOR @ 15°C, 1.01325 bar	Note	Reference	-SECOND VIRIAL COEFFICIENT @ 15°C / $cm^3\ mol^{-1}$	Reference	IDEAL RELATIVE DENSITY	REAL GAS RELATIVE DENSITY @ 0°C, 1.01325 bar	Note	REAL GAS RELATIVE DENSITY @ 15°C, 1.01325 bar	Note
1	METHANE	0.9976		ARM	0.9980		ARM	47.0	ARM	0.5539	0.5549		0.5548	
2	ETHANE	0.9900		ARM	0.9915		ARM	199.1	ARM	1.0382	1.0481		1.0467	
3	PROPANE	0.9789		ARM	0.9821		ARM	415	ARM	1.5225	1.5544		1.5496	
4	n-BUTANE	0.9572		ARM	0.9650		ARM	799	ARM	2.0069	2.0953		2.0788	
5	2-METHYLPROPANE	0.958		ARM	0.968		ARM	738	ARM	2.0069	2.094		2.072	
6	n-PENTANE	0.918	h	ARM	0.937	h	ARM	1398	ARM	2.4912	2.712	h	2.658	h
7	2-METHYLBUTANE	0.937	h	ARM	0.948	h	ARM	1170	ARM	2.4912	2.657	h	2.627	h
8	2,2-DIMETHYLPROPANE	0.943	h	ARM	0.955		ARM	1027	ARM	2.4912	2.640	h	2.607	
9	n-HEXANE	0.892	h	PZC	0.913	h	PZC	2053	PZC	2.9755	3.334	h	3.258	h
10	2-METHYLPENTANE	0.898	h	ARM	0.914	h	ARM	1853	ARM	2.9755	3.311	h	3.254	h
11	3-METHYLPENTANE	0.898	h	ARM	0.917	h	ARM	1809	ARM	2.9755	3.311	h	3.243	h
12	2,2-DIMETHYLBUTANE	0.916	h	PZC	0.931	h	PZC	1626	PZC	2.9755	3.246	h	3.195	h
13	2,3-DIMETHYLBUTANE	0.910	h	ARM	0.925	h	ARM	1634	ARM	2.9755	3.268	h	3.215	h
14	n-HEPTANE	0.830	h	PZC	0.866	h	PZC	3165	PZC	3.4598	4.166	h	3.993	h
15	n-OCTANE	0.742	h	PZC	0.802	h	PZC	4687	PZC	3.9441	5.312	h	4.916	h
16	n-NONANE	0.613	h	PZC	0.710	h	PZC	6855	PZC	4.4284	7.220	h	6.235	h
17	n-DECANE	0.434	h	PZC	0.584	h	PZC	9826	PZC	4.9127	11.313	h	8.409	h
18	ETHENE	0.9925		ARM	0.9936		ARM	150.3	ARM	0.9686	0.9754		0.9745	
19	PROPENE	0.981		ARM	0.984		ARM	373	ARM	1.4529	1.480		1.476	
20	1-BUTENE	0.965		PZC	0.970		PZC	702	PZC	1.9372	2.006		1.996	
21	cis-2-BUTENE	0.961	h	PZC	0.967		PZC	772	PZC	1.9372	2.015	h	2.003	
22	trans-2-BUTENE	0.961	h	PZC	0.968		PZC	768	PZC	1.9372	2.015	h	2.000	
23	2-METHYLPROPENE	0.965		PZC	0.971		PZC	699	PZC	1.9372	2.006		1.994	
24	1-PENTENE	0.938	h	PZC	0.949	h	PZC	1205	PZC	2.4216	2.580	h	2.551	h
25	PROPADIENE	0.980		PZC	0.983		PZC	405	PZC	1.3833	1.411		1.407	
26	1,2-BUTADIENE	0.955	h	PZC	0.963		PZC	879	PZC	1.8676	1.954	h	1.939	
27	1,3-BUTADIENE	0.966		PZC	0.971		PZC	677	PZC	1.8676	1.932		1.923	

28	ETHYNE	0.991		TWT	0.993		TWT	171	PZC	0.8990	0.907		0.905	
29	CYCLOPENTANE	0.935	h	PZC	0.947	h	PZC	1248	PZC	2.4216	2.588	h	2.556	h
30	METHYLCYLOPENTANE	0.902	h	PZC	0.921	h	PZC	1860	PZC	2.9059	3.220	h	3.154	h
31	ETHYLCYCLOPENTANE	0.841	h	PZC	0.876	h	PZC	2938	PZC	3.3902	4.029	h	3.868	h
32	CYCLOHEXANE	0.897	h	PZC	0.918	h	PZC	1936	PZC	2.9059	3.238	h	3.164	h
33	METHYLCYCLOHEXANE	0.855	h	PZC	0.886	h	PZC	2699	PZC	3.3902	3.963	h	3.825	h
34	ETHYLCYCLOHEXANE	0.770	h	PZC	0.824	h	PZC	4167	PZC	3.8745	5.029	h	4.700	h
35	BENZENE	0.909	h	ARM	0.926	h	ARM	1613	ARM	2.6971	2.965	h	2.911	h
36	TOLUENE	0.849	h	PZC	0.883	h	PZC	2770	PZC	3.1814	3.745	h	3.601	h
37	ETHYLBENZENE	0.764	h	PZC	0.823	h	PZC	4197	PZC	3.6657	4.795	h	4.452	h
38	o-XYLENE	0.737	h	PZC	0.804	h	PZC	4628	PZC	3.6657	4.971	h	4.557	h
39	METHANOL	0.773	h	TSO	0.872	h	TSO	2633	TSO	1.1063	1.430	h	1.268	h
40	METHANETHIOL	0.972	h	PZC	0.977		PZC	547	PZC	1.6611	1.708	h	1.699	
41	HYDROGEN	1.0006		ARM	1.0006		ARM	-14.0	ARM	0.06960	0.06952		0.06953	
42	WATER	0.930	h	ARM	0.945	h	ARM	1224	ARM	0.6220	0.668	h	0.658	h
43	HYDROGEN SULPHIDE	0.990		LNZ	0.990		LNZ	229	LNZ	1.1768	1.188		1.188	
44	AMMONIA	0.985		HAG	0.988		HAG	282	HAG	0.5880	0.597		0.595	
45	HYDROGEN CYANIDE	0.887	h	EXT	0.912	h	EXT	1900	EXT	0.9331	1.051	h	1.023	h
46	CARBON MONOXIDE	0.9993		HIL	0.9995		HIL	10.5	DYS	0.9671	0.9672		0.9672	
47	CARBONYL SULPHIDE	0.985		PZC	0.987		PZC	298	PZC	2.0743	2.107		2.101	
48	CARBON DISULPHIDE	0.954	h	EXT	0.962	h	DYS	875	DYS	2.6290	2.754	h	2.733	
49	HELIUM	1.0005		ARM	1.0005		ARM	-11.9	ARM	0.1382	0.1380		0.1381	
50	NEON	1.0005		DYS	1.0005		DYS	-11.2	DYS	0.6967	0.6960		0.6961	
51	ARGON	0.9990		ARM	0.9992		ARM	18.2	ARM	1.3793	1.3799		1.3798	
52	NITROGEN	0.9995		ARM	0.9997		ARM	7.1	ARM	0.9672	0.9671		0.9671	
53	OXYGEN	0.9990		ARM	0.9992		ARM	18.4	ARM	1.1048	1.1053		1.1053	
54	CARBON DIOXIDE	0.9933		ARM	0.9944		ARM	132.3	ARM	1.5195	1.5289		1.5275	
55	SULPHUR DIOXIDE	0.976		LNZ	0.979		LNZ	484	LNZ	2.2120	2.264		2.258	
	AIR	0.99941		HIL	0.99958		HIL	10.1	ARM	1.0000	1.0000		1.0000	

TABLE 4

ENTHALPIES OF FORMATION AND COMBUSTION

		-STANDARD ENTHALPY OF FORMATION @ 25°C / kJ mol^{-1}	Reference	-STANDARD ENTHALPY OF COMBUSTION @ 25°C / kJ mol^{-1}	Reference	-STANDARD ENTHALPY OF COMBUSTION @ 15°C / kJ mol^{-1}	Reference	-REAL GAS ENTHALPY OF COMBUSTION @ 25°C, 1.01325 bar / kJ mol^{-1}	Note	-REAL GAS ENTHALPY OF COMBUSTION @ 15°C, 1.01325 bar / kJ mol^{-1}	Note	-REAL GAS ENTHALPY OF COMBUSTION @ 0°C, 1.01325 bar / kJ mol^{-1}	Note	Reference
1	METHANE	74.52	TRC.85	890.65	GAR	891.58	GAR	890.66		891.59		893.00		LNG
2	ETHANE	83.82	TRC.85	1560.69	GAR	1562.14	GAR	1560.7		1562.1		1564.3		LNG
3	PROPANE	104.68	TRC.85	2219.17	GAR	2221.10	GAR	2219.1		2221.0		2223.9		LNG
4	n-BUTANE	125.79	TRC.85	2877.40	GAR	2879.76	GAR	2877.2		2879.5		2883.0		LNG
5	2-METHYLPROPANE	134.99	TRC.85	2868.20	GAR	2870.58	GAR	2868.1		2870.4		2874.0		LNG
6	n-PENTANE	146.76	TRC.85	3535.77	GAR	3538.60	GAR		ℓ		ℓ		ℓ	
7	2-METHYLBUTANE	153.70	TRC.85	3528.83	GAR	3531.68	GAR		ℓ		ℓ		ℓ	
8	2,2-DIMETHYLPROPANE	167.92	TRC.85	3514.61	GAR	3517.43	GAR	3514.4		3517.1			ℓ	LNG
9	n-HEXANE	166.92	TRC.85	4194.95	GAR	4198.24	GAR		ℓ		ℓ		ℓ	
10	2-METHYLPENTANE	174.55	TRC.85	4187.32	GAR	4190.62	GAR		ℓ		ℓ		ℓ	
11	3-METHYLPENTANE	171.97	TRC.85	4189.90	GAR	4193.22	GAR		ℓ		ℓ		ℓ	
12	2,2-DIMETHYLBUTANE	184.35	AEH	4177.52	GAR	4180.83	GAR		ℓ		ℓ		ℓ	
13	2,3-DIMETHYLBUTANE	176.59	AEH	4185.28	GAR	4188.60	GAR		ℓ		ℓ		ℓ	
14	n-HEPTANE	187.78	TRC.84	4853.43	TRC.84	4857.18	HUM		ℓ		ℓ		ℓ	
15	n-OCTANE	208.75	TRC.85	5511.80	TRC.84	5516.01	HUM		ℓ		ℓ		ℓ	
16	n-NONANE	228.74	TRC.84	6171.15	TRC.84	6175.82	HUM		ℓ		ℓ		ℓ	
17	n-DECANE	249.46	TRC.84	6829.77	TRC.84	6834.90	HUM		ℓ		ℓ		ℓ	
18	ETHENE	-52.50	AEH	1411.18	GAR	1412.11	GAR	1411.19		1412.13		1413.54		HUM
19	PROPENE	-20.00	AEH	2058.02	GAR	2059.43	GAR	2058.0		2059.4		2061.5		HUM
20	1-BUTENE	0.54	TRC.83	2716.82	AEH	2718.70	HUM	2716.8		2718.6		2721.5		HUM
21	cis-2-BUTENE	7.4	TRC.83	2710.0	TRC.83	2711.9	HUM	2709.9		2711.9			ℓ	HUM
22	trans-2-BUTENE	11.0	TRC.83	2706.4	TRC.83	2708.3	HUM	2706.3		2708.2			ℓ	HUM
23	2-METHYLPROPENE	17.1	TRC.83	2700.2	TRC.83	2702.0	HUM	2700.2		2702.0		2704.8		HUM
24	1-PENTENE	21.28	TRC.83	3375.42	AEH	3377.75	HUM		ℓ		ℓ		ℓ	
25	PROPADIENE	-190.92	TRC.84	1943.11	AEH	1943.96	HUM	1943.1		1944.0		1945.2		HUM
26	1,2-BUTADIENE	-162.26	TRC.84	2593.79	AEH	2595.12	HUM	2593.7		2595.1			ℓ	HUM
27	1,3-BUTADIENE	-109.24	TRC.84	2540.77	AEH	2542.10	HUM	2540.7		2542.1		2544.1		HUM

28	ETHYNE	-228.20	AEH	1301.05	GAR	1301.37	GAR	1301.1	1301.4	1301.9	HUM
29	CYCLOPENTANE	77.11	AEH	3319.59	GAR	3322.19	GAR	ℓ	ℓ	ℓ	
30	METHYLCYCLOPENTANE	106.60	AEH	3969.44	TRC.66	3972.46	HUM	ℓ	ℓ	ℓ	
31	ETHYLCYCLOPENTANE	126.91	AEH	4628.47	TRC.66	4631.95	HUM	ℓ	ℓ	ℓ	
32	CYCLOHEXANE	123.08	AEH	3952.96	GAR	3956.02	GAR	ℓ	ℓ	ℓ	
33	METHYLCYCLOHEXANE	154.74	AEH	4600.64	TRC.66	4604.09	HUM	ℓ	ℓ	ℓ	
34	ETHYLCYCLOHEXANE	171.67	AEH	5263.05	TRC.66	5266.95	HUM	ℓ	ℓ	ℓ	
35	BENZENE	-82.88	AEH	3301.43	GAR	3302.86	GAR	ℓ	ℓ	ℓ	
36	TOLUENE	-50.00	TRC.84	3947.89	AEH	3949.81	HUM	ℓ	ℓ	ℓ	
37	ETHYLBENZENE	-29.92	TRC.84	4607.15	AEH	4609.53	HUM	ℓ	ℓ	ℓ	
38	o-XYLENE	-19.08	TRC.84	4596.31	AEH	4598.64	HUM	ℓ	ℓ	ℓ	
39	METHANOL	201.08	WIL	764.09	WIL	765.09	HUM	ℓ	ℓ	ℓ	
40	METHANETHIOL	22.59	TRC.81	1239.39	AEH	1240.28	HUM	1239.4	1240.3	ℓ	HUM
41	HYDROGEN	0		285.83	COD	286.15	HUM	285.83	286.14	286.63	HUM
42	WATER	241.814	COD	44.016	COD	44.433	HUM	ℓ	ℓ	ℓ	
43	HYDROGEN SULPHIDE	20.63	NBS	562.01	AEH	562.38	HUM	562.0	562.4	563.0	HUM
44	AMMONIA	45.94	COD	382.81	AEH	383.51	HUM	382.8	383.4	384.5	HUM
45	HYDROGEN CYANIDE	-135.1	NBS	671.5	AEH	671.7	HUM	ℓ	ℓ	ℓ	
46	CARBON MONOXIDE	110.53	COD	282.98	AEH	282.91	HUM	283.01	282.94	282.83	HUM
47	CARBONYL SULPHIDE	142.09	NBS	548.23	AEH	548.15	HUM	548.3	548.2	548.1	HUM
48	CARBON DISULPHIDE	-117.36	NBS	1104.49	AEH	1104.32	HUM	ℓ	ℓ	ℓ	
49	HELIUM	0		0		0		0	0	0	
50	NEON	0		0		0		0	0	0	
51	ARGON	0		0		0		0	0	0	
52	NITROGEN	0		0		0		0	0	0	
53	OXYGEN	0		0		0		0	0	0	
54	CARBON DIOXIDE	393.51	COD	0		0		0	0	0	
55	SULPHUR DIOXIDE	296.81	COD	0		0		0	0	0	

TABLE 5

CALORIFIC VALUES

		IDEAL GAS GROSS CALORIFIC VALUE / MJ m^{-3}			REAL-GAS GROSS CALORIFIC VALUE / MJ m^{-3}						REAL-GAS GROSS CALORIFIC VALUE / MJ kg^{-1} @ 25°C, 1.01325 bar	
		(1) Combustion @ 25°C Metered @ 0°C	(2) Combustion @ 15°C Metered @ 0°C	(3) Combustion @ 15°C Metered @ 15°C	(1) Combustion @ 25°C Metered @ 0°C, 1.01325 bar	Note	(2) Combustion @ 15°C Metered @ 0°C, 1.01325 bar	Note	(3) Combustion @ 15°C Metered @ 15°C, 1.01325 bar	Note		Note
1	METHANE	39.736	39.778	37.707	39.832		39.874		37.783		55.518	
2	ETHANE	69.63	69.69	66.07	70.33		70.40		66.63		51.90	
3	PROPANE	99.01	99.09	93.94	101.14		101.23		95.64		50.32	
4	n-BUTANE	128.38	128.48	121.79	134.11		134.21		126.20		49.50	
5	2-METHYLPROPANE	127.96	128.07	121.40	133.6		133.7		125.4		49.35	
6	n-PENTANE	157.75	157.87	149.66		ℓ		ℓ		ℓ		ℓ
7	2-METHYLBUTANE	157.44	157.57	149.36		ℓ		ℓ		ℓ		ℓ
8	2,2-DIMETHYLPROPANE	156.80	156.93	148.76		ℓ		ℓ	155.8		48.71	
9	n-HEXANE	187.16	187.30	177.55		ℓ		ℓ		ℓ		ℓ
10	2-METHYLPENTANE	186.82	186.96	177.23		ℓ		ℓ		ℓ		ℓ
11	3-METHYLPENTANE	186.93	187.08	177.34		ℓ		ℓ		ℓ		ℓ
12	2,2-DIMETHYLBUTANE	186.38	186.53	176.82		ℓ		ℓ		ℓ		ℓ
13	2,3-DIMETHYLBUTANE	186.73	186.87	177.15		ℓ		ℓ		ℓ		ℓ
14	n-HEPTANE	216.54	216.70	205.42		ℓ		ℓ		ℓ		ℓ
15	n-OCTANE	245.91	246.10	233.29		ℓ		ℓ		ℓ		ℓ
16	n-NONANE	275.33	275.53	261.19		ℓ		ℓ		ℓ		ℓ
17	n-DECANE	304.71	304.94	289.06		ℓ		ℓ		ℓ		ℓ
18	ETHENE	62.96	63.00	59.72	63.44		63.48		60.11		50.30	
19	PROPENE	91.82	91.88	87.10	93.6		93.7		88.5		48.91	
20	1-BUTENE	121.21	121.29	114.98	125.6		125.7		118.5		48.42	
21	cis-2-BUTENE	120.91	120.99	114.69		ℓ		ℓ	118.6		48.30	
22	trans-2-BUTENE	120.75	120.83	114.54		ℓ		ℓ	118.3		48.23	
23	2-METHYLPROPENE	120.47	120.55	114.27	124.8		124.9		117.7		48.12	
24	1-PENTENE	150.59	150.70	142.85		ℓ		ℓ		ℓ		ℓ
25	PROPADIENE	86.69	86.73	82.21	88.5		88.5		83.6		48.50	
26	1,2-BUTADIENE	115.72	115.78	109.75		ℓ		ℓ	114.0		47.95	
27	1,3-BUTADIENE	113.36	113.42	107.51	117.3		117.4		110.7		46.97	

28	ETHYNE	58.05	58.06	55.04	58.6	58.6	55.4	49.97
29	CYCLOPENTANE	148.10	148.22	140.50	ℓ	ℓ	ℓ	ℓ
30	METHYLCYCLOPENTANE	177.10	177.23	168.01	ℓ	ℓ	ℓ	ℓ
31	ETHYLCYCLOPENTANE	206.50	206.65	195.90	ℓ	ℓ	ℓ	ℓ
32	CYCLOHEXANE	176.36	176.50	167.31	ℓ	ℓ	ℓ	ℓ
33	METHYLCYCLOHEXANE	205.26	205.41	194.72	ℓ	ℓ	ℓ	ℓ
34	ETHYLCYCLOHEXANE	234.81	234.98	222.75	ℓ	ℓ	ℓ	ℓ
35	BENZENE	147.29	147.36	139.69	ℓ	ℓ	ℓ	ℓ
36	TOLUENE	176.13	176.22	167.05	ℓ	ℓ	ℓ	ℓ
37	ETHYLBENZENE	205.55	205.65	194.95	ℓ	ℓ	ℓ	ℓ
38	o-XYLENE	205.06	205.17	194.49	ℓ	ℓ	ℓ	ℓ
39	METHANOL	34.09	34.13	32.36	ℓ	ℓ	ℓ	ℓ
40	METHANETHIOL	55.30	55.34	52.45	ℓ	ℓ	53.7	25.76
41	HYDROGEN	12.752	12.767	12.102	12.745	12.758	12.094	141.79
42	WATER	1.96	1.98	1.88	ℓ	ℓ	ℓ	ℓ
43	HYDROGEN SULPHIDE	25.07	25.09	23.78	25.33	25.35	24.03	16.49
44	AMMONIA	17.08	17.11	16.22	17.34	17.37	16.41	22.47
45	HYDROGEN CYANIDE	29.96	29.97	28.41	ℓ	ℓ	ℓ	ℓ
46	CARBON MONOXIDE	12.63	12.62	11.96	12.64	12.63	11.97	10.10
47	CARBONYL SULPHIDE	24.46	24.46	23.18	24.83	24.83	23.49	9.13
48	CARBON DISULPHIDE	49.28	49.27	46.70	ℓ	ℓ	ℓ	ℓ
49	HELIUM	0	0	0	0	0	0	0
50	NEON	0	0	0	0	0	0	0
51	ARGON	0	0	0	0	0	0	0
52	NITROGEN	0	0	0	0	0	0	0
53	OXYGEN	0	0	0	0	0	0	0
54	CARBON DIOXIDE	0	0	0	0	0	0	0
55	SULPHUR DIOXIDE	0	0	0	0	0	0	0

TABLE 6

FLAMMABILITY DATA

		LOWER FLAMMABILITY LIMIT IN AIR / % v	Reference	UPPER FLAMMABILITY LIMIT IN AIR / % v	Reference	MINIMUM AUTOIGNITION TEMPERATURE / K	Note	Reference
1	METHANE	4.9	RSW	15.0	RSW	874		RSM
2	ETHANE	2.8	RSW	15.5	NAB	745		STU
3	PROPANE	2.1	RSW	9.8	RSW	723		STU
4	n-BUTANE	1.5	NAB	8.5	RSW	561		STU
5	2-METHYLPROPANE	1.8	NAB	8.5	NAB	733		STU
6	n-PENTANE	1.4	BUR	8.3	ESD	516		STU
7	2-METHYLBUTANE	1.3	NAB	8.0	ESD	693		STU
8	2,2-DIMETHYLPROPANE	1.3	NAB	7.5	NAB	723		STU
9	n-HEXANE	1.2	BUR	7.7	ESD	498		STU
10	2-METHYLPENTANE	1.2	NAB	7.0	NAB	537		STU
11	3-METHYLPENTANE	1.2	NAB	7.0	NAB	551		STU
12	2,2-DIMETHYLBUTANE	1.2	NAB	7.0	NAB	678		STU
13	2,3-DIMETHYLBUTANE	1.2	NAB	7.0	NAB	669		STU
14	n-HEPTANE	1.1	BUR	7.0	ESD	477		STU
15	n-OCTANE	0.95	BUR	6.5	NAB	479		STU
16	n-NONANE	0.84	BUR	5.6	NAB	478		STU
17	n-DECANE	0.77	BUR	5.4	NAB	474		STU
18	ETHENE	2.7	ZAB	36	ZAB	698		NAB
19	PROPENE	2.0	NAB	11.7	NAB	728		STU
20	1-BUTENE	1.6	NAB	10	NAB	658		STU
21	cis-2-BUTENE	1.7	GAZ	9.7	GAZ	598		STU
22	trans-2-BUTENE	1.7	GAZ	9.7	GAZ	598		STU
23	2-METHYLPROPENE	1.8	GAZ	9.6	GAZ	738		STU
24	1-PENTENE	1.3	ESD	10.0	ESD	548		STU
25	PROPADIENE	2.2	ZAB	11.7	ESD			
26	1,2-BUTADIENE	1.6	ESD	10.3	ESD			
27	1,3-BUTADIENE	1.1	NAB	12.5	NAB	688		NAB

28	ETHYNE	1.5	NAB	100	NAB	578	NAB
29	CYCLOPENTANE	1.5	ESD	8.3	ESD	634	STU
30	METHYLCYCLOPENTANE	1.0	ESD	8.4	ESD	531	STU
31	ETHYLCYCLOPENTANE	1.1	NAB	6.7	NAB	533	STU
32	CYCLOHEXANE	1.2	NAB	8.3	NAB	518	STU
33	METHYLCYCLOHEXANE	1.1	ZAB	6.7	ZAB	523	ZAB
34	ETHYLCYCLOHEXANE	0.9	NAB	6.6	NAB	511	STU
35	BENZENE	1.2	NAB	8.0	NAB	771	STU
36	TOLUENE	1.2	ZAB	7.1	ZAB	753	STU
37	ETHYLBENZENE	1.0	NAB	7.8	NAB	703	NAB
38	o-XYLENE	1.0	NAB	7.6	NAB	737	STU
39	METHANOL	5.5	NAB	44	NAB	658	STU
40	METHANETHIOL	3.9	GAZ	21.8	GAZ		
41	HYDROGEN	4.0	NAB	75.6	NAB	673	ZAB
42	WATER	0		0		n	
43	HYDROGEN SULPHIDE	4.0	ZAB	45.5	NAB	543	NAB
44	AMMONIA	15	NAB	28	NAB	903	NAB
45	HYDROGEN CYANIDE	5.4	NAB	46.6	NAB	808	NAB
46	CARBON MONOXIDE	12.5	NAB	74	NAB	878	NAB
47	CARBONYL SULPHIDE	11.9	NAB	29	NAB		
48	CARBON DISULPHIDE	1.0	NAB	60	NAB	363	ZAB
49	HELIUM	0		0		n	
50	NEON	0		0		n	
51	ARGON	0		0		n	
52	NITROGEN	0		0		n	
53	OXYGEN	0		0		n	
54	CARBON DIOXIDE	0		0		n	
55	SULPHUR DIOXIDE	0		0		n	