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# Refrigerants of the Methane, Ethane and Propane Series: Thermal Conductivity Calculation Along the Saturation Line

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## ABSTRACT

In this paper a formula is presented for the calculation of thermal conductivity of liquids along the saturation line.
The formula is valid for organic compounds in a wide reduced temperature range (*0.30* to *0.95*), but is proven to be particularly reliable for refrigerants by testing it on a database of more than 40 refrigerants of the methane, ethane and propane series that includes almost all those reported by ASHRAE in its 2007 revision of standard 34.
The test on the indicated refrigerants shows a very satisfying performance: mean and maximum absolute deviations between calculated values and experimental data are generally less than *3%* and *8%* respectively.
The proposed formula is very simple: three characteristic parameters appear in the equation to express the thermal conductivity dependence on the reduced temperature: the constant "$\Phi$", a multiplying factor "$A$", and an exponent "$a$".

## 1. INTRODUCTION

Thermal conductivity is a property required in all heat transfer problems. It appears as the parameter $\lambda$ (W m$^{-1}$ K$^{-1}$) in the well known "Fourier's law" (Fourier, 1822) describing thermal conduction in a mono-dimensional flow through a section of infinitesimal area $dA$, normal to the direction $x$ of the flow.

$$dq = -\lambda \cdot dA \frac{dT}{dx} \tag{1}$$

Thermal conductivity is a characteristic of each compound, depending on the molecular structure. Most organic liquids (therefore almost all refrigerants) show thermal conductivity values in the range 0.100÷0.200 W m$^{-1}$ K$^{-1}$; simple liquids thermal conductivity is usually 10 to 100 times those of the same substances in the gaseous state and 0.1÷0.2 times those of the corresponding solid near the normal melting point.
From a theoretical point of view, thermal conductivity is a function of temperature and density; in expressions used for engineering purposes, density is usually replaced by pressure. Moreover pressure dependence is often neglected, because of its small influence at pressures under 5÷6 MPa (McLaughlin, 1964).
The knowledge of the value of thermal conductivity of a particular refrigerant is always necessary for industrial design of a refrigeration cycle and especially of some equipment in it, such as heat exchangers, pipes and vessels.

At present, from the industrial point of view, the investigation of thermal conductivity and other transport properties has grown interest; if in the past, most intense research involved the equilibrium properties, to determine the feasibility of a particolar process, today's attention on process integration and energy minimization has led to a growing interest on the non-equilibrium properties since they govern the geometrical dimensions of a machine and/or the timescale of a process (Wakeham, 1996).
In this work a formula is presented and tested on a set of more than 40 refrigerants of the methane, ethane and propane series. The most used refrigerants, especially almost all those reported by ASHRAE in its 2007 revision of standard 34 are included in the test and many recent data are used.
A wide reduced temperature range is investigated, from 0.30 to 0.95; for higher temperature values the critical enhancement appears and "liquid-state" formulas are not applicable.

## 2. THERMAL CONDUCTIVITY PREDICTION AND ESTIMATION

A wide database of measured values of thermal conductivity exists in literature, especially in the field of refrigerants, since many organic compounds have been widely used for many years. Also, a great amount of experimental data on new refrigerants has been produced after the adoption of the Montreal Protocol on Substances that Deplete the Ozone Layer.
Nevertheless, the efforts for producing experimental data doesn't reduce the necessity of formulas and models to generate values where there are no experimental ones: Nieto de Castro and Wakeham (1996) highlighted the importance of correlation, estimation and prediction with considerations on the large time that would be necessary to measure all the values of only the most important properties generally involved in process design for the most frequently used chemicals.
For this reason prediction, estimation and correlation methods have been widely used for the generation of values of transport properties; correlation methods can be used only when a sufficient amount of data is available, and, in most cases, this is not the situation for refrigerants. The other two methods have both been used in the case of thermal conductivity, but prediction hasn't yet come to reliable results in the case of liquids due to the lack of a well-defined theory of the liquid state; so prediction methods usually need the employment of many experimental-derived parameters, becoming then estimation methods in order to produce acceptable results.
In the end reliable methods are to be found in the field of estimation, as was stated in previous works by Latini and his research team after a detailed work carried out in the early 70's (Baroncini *et al*., 1979). Even if several years have passed, the conclusion is still true.
Some empirical methods used at present for liquids are the one by Sastri the one by Chung et al. and the so-called TRAPP method (Poling et al., 2001). The method by Sastri is originally developed for liquids, while the other two were specifically devised to treat liquid systems at high reduced pressures and high-pressure gases.
A wide collection and description of other methods and a test of their performances can be found in Baroncini *et al.*, (1979).
The main problems for most formulas are the small set of substances for which each expression is reliable and the requirement of too many parameters for the formula in order to use it. Also the temperature range in which the formula is applicable, is particularly important in the filed of refrigerants, that are used under a wide temperature range inside the same equipment.

## 3. THERMAL CONDUCTIVITY'S DEPENDENCE ON TEMPERATURE AND PRESSURE

Thermal conductivity of liquids depends upon temperature and pressure. In the liquid state thermal conductivity usually decreases with the increase of temperature, but there are some exceptions to this behavior like water and some aqueous solutions. Thermal conductivity dependence on temperature under the normal boiling point or next to it is usually linear; in this area $\lambda$ can be represented as:

$$\lambda = \lambda_0 - BT \tag{2}$$

Linearity ceases moving away from the normal boiling point. Regarding the dependence on density, thermal conductivity generally increases with the increase of density; for engineering purposes, and also for measuring difficulties, density is usually substituted by pressure; variations of thermal conductivity with pressure are irrelevant

up to pressures of 5 ÷ 6 MPa (Poling at al., 2001). The critical point represents a singularity and there is a very particular behavior next to it. For pressure values higher than 50 MPa there is an inversion of the effect of pressure.

## 4. FORMULA BY LATINI et al.

### 4.1 Previous formulas

Latini and his group started their research on thermal conductivity in the 1970's. At the beginning Visvanath's equation was used as a starting point to develop more accurate correlations.
The correlation produced expresses thermal conductivity of organic liquids along the saturation line as a function of temperature (Baroncini *et al.,* 1981)

$$\lambda = A\frac{(1-T_r)^{0.38}}{T_r^{\frac{1}{6}}} \tag{3}$$

$A$ is the value of the thermal conductivity at the reduced temperature $T_r \approx 0.55$. Equation 3 has become a reference, reported by Poling *et al.* (2001). Errors of this formula are usually less than 10% in the range $T_r = 0.3 \div 0.8$. Later the formula has been revised and the following expression has been presented (Latini and Polonara, 2007):

$$\lambda = A\left[\frac{(1-T_r)^2}{T_r}\right]^a \tag{4}$$

Parameter $a$ assumes rational values less than 1, and each value is typical of one family of compounds (alkanes, alkenes, refrigerants of the methane serie, refrigerants of the ethane serie, etc.), while $A$ is calculated with experimental data for each liquid. The new expression has a particular peculiarity: when the expression in brackets equals 1, $A=\lambda(T_r \approx 0.3820)$. Parameter $A$ is therefore the value of thermal conductivity of the liquid at a precise temperature, that is when:

$$\frac{1-T_r}{T_r} = \frac{1+\sqrt{5}}{2} \cong 1.6180339887... \tag{5}$$

In this way the golden ratio ($\Phi$), i.e. the well known number linked to the Fibonacci's sequence ($F$=1 ,1 ,2 ,3 ,5 ,8 ,13 ,21 ,34 ,55 ,89 ,144 , …) is shown to be in a special relation with the liquid state.

$$\lim_{n\to\infty}\frac{F_{(n+1)}}{F_{(n)}} = \frac{\sqrt{5}+1}{2} = 1.6180339887... = \Phi \tag{6}$$

Tests have been performed on the formula, showing a good behavior: thermal conductivity values along the saturation line in the range $T_r = 0.3 \div 0.8$ show mean absolute errors less than 2%. Also the simplicity of the formula and the wide temperature range of application are worth being pointed out.

### 4.2 The proposed formula

Since 2007 new improvements have been made on the formula, having three particular aims:

- further investigating the relation between the liquid state and the special number called "golden ratio";
- proposing a formula reliable for an very large set of fluids;
- testing the formula on a wide temperature field, possibly covering all the range usually needed in engineering for process design;

The first of these aims led to a slight modification of the 2007 expression, to more clearly express the link between the relation and the golden ratio (Latini, 2009):

$$\lambda = A\left[\sqrt{5}\,\frac{(\Phi - T_r)^2}{\Phi + T_r}\right]^a \tag{6}$$

Analyzing the formula, it is immediately evident that:

$$A = \lambda(T_r = \Phi - 1) \tag{9}$$

*A* has a precise physical meaning: it is the value of the liquid's thermal conductivity at a reduced temperature value of 0.6180339887 …, the mantissa of the golden ratio. As in the previous cases, "*a*" assumes one value for each serie of organic liquids, chosen experimentally in the set of rational numbers less than 1.

## 5. EXTENSIVE TEST OF THE FORMULA ON REFRIGERANT FLUIDS

The steps of the formula's test are described in the following subsections; at the end, the results of the test are shown.

### 5.1 Investigated refrigerants

The presented formula claims the possibility of application in process and apparatuses design engineering; for this reason, the main interest is to find out whether or not it is reliable in the case of major chemicals; especially common refrigerants, that are the substances the formula is meant for. For this reason ASHRAE Standard 34 was chosen for the definition of a list refrigerants on which the formula should be tested because the standard is in continuous maintenance: refrigerants no longer in use are deleted, and new refrigerants are added to keep up with the present industrial applications.

Only 4 refrigerants included in Standard 34 are not in the present study (i.e. R40, R41, R 227ea and R245fa), since reliable measures weren't available.

Other than those in Standard 34, also some refrigerants commonly used in the past, for which measures where available from earlier studies, have been included in the database. In conclusion, investigated liquids are a total of 42, of which 15 belong to the methane serie refrigerants, 22 to the ethane serie and 5 to the propane serie.

Some notes should be reported about the measures used:

- the investigated temperature range is very wide, going from $T_r$=0.3 to $T_r$=0.95; almost in every case this range covers the entire field of application of the refrigerant, since lower and higher temperatures are unlikely to be used. Regarding high temperatures, the critical enhancement doesn't allow to go any closer to the critical point. Of course, not in all cases experimental values are available in the entire $T_r$ range;
- only experimental values have been used in the test; when possible, also, the original "experimental" reference is reported; when this wasn't possible, the handbook or the database where values were found are reported;
- in some cases, the saturated liquid value wasn't available: for those refrigerants, also values at atmospheric or "low"(less than 5 or 6 MPa) pressure have been adopted;
- when possible, recent data where adopted, since it is proved that they are more reliable than old ones; especially since the 70's, modern measurement techniques have improved accuracy of measurements, and old measures have big errors (the case of Toluene is reported by Wakeham, (1996));
- the information about the kind of apparatus measures were taken by wasn't available in many cases; for this reason this information is not reported;
- in almost all cases values from different sources have been mixed; even if an uncertainty range is often declared, in many cases differences between different sets are out of the declared range and contribute to the overall error.

### 5.2 Formula's application

In order to generate a thermal conductivity value for a specified temperature by using the proposed formula, some information about the refrigerant in object is needed:

- the reduced temperature value, which means that the critical temperature of the given refrigerant has to be known;
- the value of the a exponent, that is characteristic of the family the substance belongs to;
- the value of the *A* parameter, i.e. the value of thermal conductivity of the refrigerant at $T_r = \Phi - 1$;

$T_c$ values used for the calculation of the reduced temperature, come from two different sources: the handbook by Poling et Al. (2001) and the "NIST Webbook" online database.
The "*a*" exponent is chosen once for every family as the value that generates the best overall fit of the formula on the considered serie of refrigerants; it is always a rational value less than one. Adopted values are reported in table 4.
The value of A in the present study has been determined by linear regression on the two measures containing the just specified $T_r$ value, when available, or by the least squares method on all the available data, when there where no points higher and lower than the specified $T_r$.

### 5.3 Test results

The results of the test are reported in table 1 through 4; information reported is the following:

- temperature range: the maximum and minimum reduced temperature for which experimental thermal conductivity values are present are expressed;
- value of the "*A*" parameters, i.e. $\lambda(T_r=\Phi-1)$;
- average percent error between experimental and calculated values, calculated as the average on all single values' errors ($100\cdot|\lambda_{cal}-\lambda_{exp}|\cdot\lambda_{cal}^{-1}$);
- maximum percent error: the maximum percent error on all the considered points;
- critical temperature: this value is very important since it is the one used to calculate the reduced temperatures from the absolute ones;
- # of experimental points;
- references;

An important consideration should be drawn about the temperature range: generally the temperature range with available measures are sufficiently wide and they cover almost the entire formula's temperature field; widest ranges are in the case of the methane serie, where 9 out of 15 refrigerants show measures in a range wider than $T_r$=0.45÷0.90; also wide ranges are for the case of the ethane serie, while for the propane serie refrigerants temperature ranges are narrower. The dimension of the range has big influence on the formula's performance, since errors tend to grow as temperature fars from the *A* value: for this reason, if the temperature range considered is narrow, errors are small; this doesn't necessarily mean that the formula performs well on the specified compound. This is the cases of alkanes (methane, ethane and propane): maximum and average errors are big, but this is mainly due the fact that temperature ranges for those substances are wider than the average of the serie.
It is also possible to notice that for measures covering the entire range considered, usually $\Delta_{max}=3\,\Delta_m$.
Maximum errors are generally measured for high reduced temperatures, as in the case of R23 and R50; in particular, in the case of R50, the high average errors is due to the presence of many experimental points at high temperatures.
In the case of refrigerants of the ethane serie, considerations are about the same; one note has to be drawn about R150 and R160B1; those two refrigerants have to be considered outliers: in fact they show very high errors for narrow temperature ranges.
In the ethane serie, it is also due reporting the case of R134a: for this refrigerants a great amount of experimental data is available, due to the very frequent use of it as a substituent of R11 and R12 that were commonly used in centrifugal compressors and domestic appliances or automotive refrigeration.
In the case of the propane serie refrigerants: small errors are influenced by the reduced number of experimental data and the narrow temperature ranges.

**Table 1: Refrigerants of the methane serie**

| ASHRAE Name | $T_{rmin}$ | $T_{rmax}$ | A | $\Delta_m$ (%) | $\Delta_{max}$ (%) | $T_c$ (K) | # of points | references |
|---|---|---|---|---|---|---|---|---|
| R10 | 0,45 | 0,84 | 0,093 | 1,15 | 2,85 | 556,30 | 23 | Vargaftik *et al.*, 1994; |
| R11 | 0,37 | 0,93 | 0,091 | 2,95 | 8,65 | 471,10 | 40 | Vargaftik *et al.*, 1994; Assael *et al.*, 1992;, Shankland, 1990; Yata *et al.*, 1984 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| R12 | 0,31 | 0,94 | 0,088 | 1,93 | 7,21 | 385,10 | 50 | Vargaftik *et al.*, 1994; Assael *et al.*, 1992; Shankland, 1990; Yata *et al.*, 1984 |
| R12B1 | 0,48 | 0,87 | 0,078 | 1,84 | 6,55 | 426,90 | 17 | Vargaftik et al., 1994 |
| R13 | 0,33 | 0,90 | 0,092 | 2,56 | 9,29 | 301,84 | 15 | Vargaftik et al., 1994; Yata *et al.*, 1984 |
| R13B1 | 0,33 | 0,95 | 0,077 | 1,36 | 3,54 | 340,15 | 30 | Vargaftik *et al.*, 1994; Yata *et al.*, 1984 |
| R14 | 0,40 | 0,67 | 0,097 | 2,71 | 4,01 | 227,51 | 14 | Zaporozhan and Geller, 1977 |
| R20 | 0,50 | 0,63 | 0,111 | 3,40 | 7,03 | 536,50 | 8 | Vargaftik *et al.*, 1994 |
| R21 | 0,45 | 0,91 | 0,106 | 0,74 | 2,21 | 451,52 | 15 | Vargaftik *et al.*, 1994 |
| R22 | 0,31 | 0,93 | 0,116 | 2,20 | 9,21 | 369,28 | 55 | Vargaftik *et al.*, 1994;, Assael *et al.*, 1992; Shankland, 1990; Yata *et al.*, 1984; Zaporozhan and Geller, 1977; Bivens *et al.,*1994 |
| R23 | 0,41 | 0,94 | 0,139 | 3,06 | 10,84 | 298,97 | 28 | Vargaftik *et al.,*1994;, Geller et al., 1993 |
| R30 | 0,37 | 0,61 | 0,134 | 2,80 | 6,53 | 510,00 | 13 | Vargaftik *et al.*, 1994 |
| R31 | 0,40 | 0,67 | 0,150 | 0,35 | 0,83 | 430,00 | 7 | Tauscher, 1969 |
| R32 | 0,43 | 0,93 | 0,192 | 1,81 | 6,13 | 351,26 | 28 | Bivens *et al.*, 1994, Tauscher, 1969; Papadaki and Wakeham, 1993 |
| R50 | 0,52 | 0,94 | 0,175 | 4,76 | 15,40 | 190,56 | 25 | Vargaftik *et al.*, 1994; Mardolcar and Nieto de Castro, 1987; Roder, 1984 |

**Table 2: Refrigerants of the ethane serie**

| **ASHRAE Name** | $T_{rmin}$ | $T_{rmax}$ | **A** | $\Delta_m$ **(%)** | $\Delta_{max}$ **(%)** | $T_c$ **(K)** | **# of points** | **references** |
|---|---|---|---|---|---|---|---|---|
| R112 | 0,54 | 0,67 | 0,075 | 1,28 | 2,31 | 551,00 | 8 | Tauscher, 1969; |
| R113 | 0,50 | 0,93 | 0,073 | 3,05 | 9,22 | 487,40 | 23 | Vargaftik *et al.*, 1994; Yata *et al.*, 1984 |
| R114 | 0,46 | 0,92 | 0,073 | 1,16 | 6,30 | 418,90 | 27 | Shankland, 1990; Geller *et al.*, 1972 |
| R114B2 | 0,58 | 0,79 | 0,061 | 1,75 | 4,51 | 487,80 | 6 | Yata *et al.*, 1984 |
| R115 | 0,48 | 0,94 | 0,076 | 1,21 | 5,03 | 353,10 | 27 | Vargaftik *et al.*, 1994; Yata *et al.*, 1984; Hahne *et al.*, 1989 |
| R116 | 0,61 | 0,89 | 0,084 | 1,13 | 1,67 | 293,04 | 5 | Tauscher, 1969 |
| R123 | 0,35 | 0,78 | 0,082 | 1,49 | 5,36 | 456,90 | 63 | Shankland, 1990; Gross *et al.*, 1990; Gross *et al.*, 1992; Yata *et al.*, 1989; Assael and Karagiannidis, 1993; Tsvetkov *et al.*, 1994 |
| R123a | 0,67 | 0,74 | 0,079 | 2,76 | 3,94 | 461,70 | 8 | Shankland, 1990 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| R124 | 0,59 | 0,93 | 0,087 | 0,97 | 3,55 | 395,60 | 22 | Yata *et al.*, 1984; Yata *et al.*, 1992; Shankland, 1990 |
| R125 | 0,51 | 0,95 | 0,098 | 3,58 | 11,57 | 339,33 | 38 | Shankland, 1990; Wilson *et al.*, 1992; Papadaki and Wakeham, 1993 |
| R130 | 0,43 | 0,57 | 0,085 | 1,37 | 2,27 | 644,50 | 10 | Vargaftik *et al.*, 1994 |
| R132b | 0,55 | 0,65 | 0,094 | 2,31 | 4,69 | 493,15 | 6 | Tauscher, 1969 |
| R133a | 0,39 | 0,72 | 0,100 | 1,24 | 3,20 | 432,02 | 8 | Tauscher, 1969 |
| R134a | 0,45 | 0,95 | 0,113 | 2,07 | 9,94 | 374,26 | 122 | Assael and Karagiannidis, 1993; Gross *et al.*, 1992; Papadaki *et al.*, 1993; Ross *et al.*, 1990; Laesecke *et al.*, 1992; Gross *et al.*, 1990; Shankland, 1990; Yata *et al.*, 1989; Perkins *et al.*, 1992; Oliveira *et al.*, 1992; Tsetkov *et al.*, 1994; Bivens *et al.*, 1994 |
| R14Assael et al., 1992; | 0,50 | 0,82 | 0,094 | 2,05 | 8,69 | 477,35 | 16 | Papadaki *et al.*, 1993; Yata *et al.*, 1992 |
| R142b | 0,54 | 0,93 | 0,097 | 0,89 | 3,40 | 410,30 | 21 | Yata *et al.*, 1992; Sousa *et al.*, 1992; Kim *et al.*, 1993 |
| R143a | 0,68 | 0,86 | 0,109 | 2,74 | 6,11 | 346,04 | 4 | Lee *et al.*, 2001; |
| R150 | 0,40 | 0,65 | 0,083 | 9,70 | 19,84 | 561,00 | 22 | Yata *et al.*, 1992; Gross *et al.*, 1992; Kim *et al.*, 1993 |
| R150B2 | 0,48 | 0,63 | 0,090 | 3,17 | 7,11 | 582,90 | 10 | Vargaftik *et al.*, 1994 |
| R152a | 0,58 | 0,94 | 0,131 | 2,85 | 4,52 | 386,41 | 22 | Yata *et al.*, 1992; Gross *et al.*, 1992; Kim *et al.*, 1993 |
| R160B1 | 0,40 | 0,62 | 0,100 | 10,07 | 19,06 | 503,80 | 12 | Vargaftik *et al.*, 1994; |
| R170 | 0,33 | 0,95 | 0,164 | 4,67 | 13,68 | 305,32 | 26 | Roder, 1984; Vargaftik *et al.*, 1994; Vesovic *et al.*, 1994 |

**Table 3: Refrigerants of the propane serie**

| ASHRAE Name | $T_{rmin}$ | $T_{rmax}$ | A | $\Delta_m$ (%) | $\Delta_{max}$ (%) | $T_c$ (K) | # of points | References |
|---|---|---|---|---|---|---|---|---|
| R218 | 0,38 | 0,93 | 0,07 | 2,73 | 5,27 | 345,10 | 20 | Vargaftik *et al.*, 1994 |
| R236fa | 0,60 | 0,95 | 0,10 | 1,12 | 2,59 | 398,10 | 13 | Gross and Song, 1996 |
| R280 | 0,56 | 0,62 | 0,11 | 1,09 | 1,76 | 503,10 | 4 | Vargaftik *et al.*, 1994 |
| R280B1fb | 0,43 | 0,61 | 0,09 | 3,22 | 5,95 | 540,45 | 11 | Vargaftik *et al.*, 1994 |
| R290 | 0,32 | 0,81 | 0,14 | 2,37 | 7,52 | 369,83 | 15 | Vargaftik *et al.*, 1994 |

**Table 4: results of the test**

| Serie | # of compounds | a | $\Delta_m$ (%) | $\Delta_{max}$ (%) |
|---|---|---|---|---|
| Methane | 15 | 0,60 | 2,24 | 6,68 |
| Ethane | 22 | 0,65 | 2,80 | 7,09 |
| Propane | 5 | 0,55 | 2,10 | 4,62 |

## 6. CONCLUSIONS

In this paper a formula for the calculation of thermal conductivity of organic liquids along the saturation line is presented and tested on a database of more than 40 refrigerants belonging to the series of methane, ethane and propane. Almost all the refrigerants present in ASHRAE Standard 34 have been considered, thus covering most of the substances in use in the refrigeration industry at the moment.
The formula is a simple expression and only one experimental points and the value of the critical temperature of the compound are needed to generate thermal conductivity values along the saturation line in the range $T_r$=0.30÷0.95.
The test shows average errors less than 2.5 % in the case of refrigerants of methane and propane series and equal to 2.8 % in the case of the propane serie. Mean maximum errors for each serie are 6.68 % in the case of the methane serie, 7.09 % in the case of ethane serie and 4.62 % in the case of the propane serie.
Only in the case of 6 compound the absolute maximum errors exceed 10%, and this generally happens when $T_r$ values are close to 0.95, and critical enhancement appears.
The results suggest that this formula can find wide technological use, due to its accuracy and simplicity.
The results showed above are extremely good especially if it is considered that errors in experimental values are rarely lower than 5%.

## NOMENCLATURE

| | | |
|---|---|---|
| $a$ | exponent in Latini's formula | |
| $A$ | multiplying factor in Latini's formula | (W m$^{-1}$ K$^{-1}$) |
| $M$ | molecular weight | (kg kmole$^{-1}$) |
| $T$ | absolute temperature | (K) |
| $T_c$ | critical temperature | (K) |
| $T_r$ | reduced temperature, $T \cdot T_c^{-1}$ | |
| $\Delta$ | percent error | (%) |
| $\Phi$ | golden ratio | |

**Subscripts**

| | |
|---|---|
| cal | calculated |
| exp | experimental |
| m | average |
| max | maximum |

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