# Reference Correlation for the Viscosity of Propane-1,2-diol (Propylene Glycol) from the Triple Point to 452 K and up to 245 MPa

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We present a new wide-ranging correlation for the viscosity of propane-1,2-diol (propylene glycol) based on critically evaluated experimental data. The correlation is designed to be used with an existing equation of state, and it is valid from the triple point of 243 K to 452 K, at pressures up to 245 MPa. The estimated uncertainty is 4.5 % (at the 95 % confidence level), except in the dilute-gas region where it is estimated to be 15 %, as there are no measurements in this region for comparison. The correlation behaves in a physically reasonable manner when extrapolated to 680 K and 350 MPa, however care should be taken when using the correlation outside of the validated range.

Key words: propane-1,2-diol; propylene glycol; transport properties; viscosity.

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## **1** Introduction

Propane-1,2-diol (IUPAC name) also known as 1,2-propanediol, propylene glycol,  $\alpha$ -propylene glycol, 1,2dihydroxypropane, or methylethylene glycol, CAS 57-55-6, C<sub>3</sub>H<sub>8</sub>O<sub>2</sub>, is employed as a heat-transfer fluid or solvent. Nevertheless, a reference correlation for its viscosity does not exist. Therefore, there is a need for a reference correlation for the viscosity of propane-1,2-diol, covering the widest possible range with the lowest possible uncertainty.

In a series of recent papers, reference correlations for the viscosity of selected common fluids [1-8], as well as very recently for ethane-1,2-diol [9], have been developed that cover a wide range of temperature and pressure conditions, including the gas, liquid, and supercritical phases. In this paper, the methodology adopted in the aforementioned papers is extended to developing a new reference correlation for the viscosity of propane-1,2-diol.

As always in such reference work, the analysis that will be described is based on the best available experimental data for the viscosity. A prerequisite to the analysis is a critical assessment of the experimental data. For this purpose, two categories of experimental data are always defined: the primary data, that are employed to develop the correlation, and the secondary data, that are used only for comparison purposes. According to the recommendation adopted by the Subcommittee on Transport Properties (now known as the International Association for Transport Properties) of the International Union of Pure and Applied Chemistry, the primary data are identified by a well-established set of criteria [10]. These criteria have been successfully employed to establish standard reference values for the viscosity and thermal conductivity of fluids over wide ranges of conditions, with uncertainties in the range of 1 %. However, in many cases, such a narrow definition unacceptably limits the range of the data representation. Consequently, sometimes within the primary data set, it is necessary to include results that extend over a wide range of conditions, albeit with a higher uncertainty, provided they are consistent with other lower uncertainty data or with theory. Nevertheless, in all cases, the uncertainty claimed for the final recommended data must reflect the estimated uncertainty in the primary information.

### 2 The Correlation

The viscosity  $\eta$  can be expressed [1-5, 7, 8] as the sum of four independent contributions, as

$$\eta(\rho, T) = \eta_0(T) + \eta_1(T)\rho + \Delta\eta(\rho, T) + \Delta\eta_c(\rho, T), \qquad (1)$$

where  $\rho$  is the density, *T* is the absolute temperature, and the first term,  $\eta_0(T) = \eta(0,T)$ , is the contribution to the viscosity in the dilute-gas limit, where only two-body molecular interactions occur. The linear-in-

density term,  $\eta_1(T) \rho$ , known as the initial density dependence term, can be separately obtained with the development of the Rainwater-Friend theory [11-13] for the transport properties of moderately dense gases. The critical enhancement term,  $\Delta \eta_c(\rho, T)$ , arises from the long-range density fluctuations that occur in a fluid near its critical point, which contribute to divergence of the viscosity at the critical point. However, this term for viscosity is significant only in the region very near the critical point, as shown in Vesovic et al. [14] and Hendl et al. [15]. Since we do not have data close to the critical point,  $\Delta \eta_c(\rho, T)$  will be set to zero in Eq. 1 and not discussed further in this work. Finally, the term  $\Delta \eta(\rho, T)$ , the residual term, represents the contribution of all other effects to the viscosity of the fluid at elevated densities including many-body collisions, molecular-velocity correlations, and collisional transfer.

The identification of these four separate contributions to the viscosity and to transport properties in general is useful because it is possible, to some extent, to treat  $\eta_0(T)$ ,  $\eta_1(T)$ , and  $\Delta \eta_c(\rho,T)$  theoretically. In addition, it is possible to derive information about both  $\eta_0(T)$  and  $\eta_1(T)$  from experiment. In contrast, there is little theoretical guidance concerning the residual contribution,  $\Delta \eta(\rho,T)$ , and therefore its evaluation is based entirely on an empirical equation obtained by fitting experimental data.

Table 1 summarizes, to the best of our knowledge, the experimental measurements of the viscosity of propane-1,2-diol reported in the literature. In the same table, the technique employed, the purity, the uncertainty as reported by the original authors, the number of measurements, as well as the range of temperatures and pressure investigated, are also shown. The commercial product is a racemic mixture, the purity is with respect to impurities.

Investigators / Reference	Year Publ.	Technique employed <sup>a</sup>	Purity <sup>b</sup> (%)	Uncertainty (%)	No. of data	Temperature range (K)	Pressure range (MPa)
Primary Data							
Azarang et al. [16]	2020	Cap	99.5	0.5	4	298-313	0.1
Miksik et al. [17]	2018	Cap	99.5	0.3	4	293-333	0.1
Sagdeev et al. [18]	2017	FCyl	99.8	1.5-2.0*	60	292-458°	0.1-245
Soldatovic et al. [19]	2016	Rcyl	99.5	2.0*	2	293, 298	0.1
Zivkovic et al. [20]	2014	Rcyl	99.0	0.8	8	288-323	0.1
Zivkovic et al. [21]	2014a	Rcyl	99.0	0.8	8	288-323	0.1
Tsai et al. [22]	2009	Cap	99.0	2.0	5	293-343	0.1
Sun and Teja [23]	2004	Cap	99.5	2.0	10	297-421	0.1
Tanaka et al. [24]	1988	FCyl	99.8	2.0	26	298, 323	0.1-118
Vinogradov and Shakhparonov [25]	1984	Cap	Purified	3.0	7	243-333	0.1
Litovitz et al. [26]	1954	Cap	na	1.5	1	293	0.1

 Table 1
 Viscosity measurements of propane-1,2-diol

Secondary Data							
Hema et al. [27]	2020	Cap	99.0	0.005	4	303-318	0.1
Trenzado et al.[28]	2020	Cap	99.5	0.4	4	288-318	0.1
Akilu et al. [29]	2019	CC	99.0	5.0	7	298-353	0.1
Esteban and Gonzalez-Miquel [30]	2018	СР	99.0	0.005*	6	298-323	0.1
Yang (Zhao) et al. [31]	2018	Cap	99.0	0.10*	6	293-318	0.1
Moosavi et al. [32]	2017	RBal	99.0	0.5*	3	293-303	0.1
Cano-Gomez et al. [33]	2017	Cap	99.5	0.05	8	298-333	0.1
Khattab et al. [34]	2017	Cap	na	0.001	7	293-323	0.1
Zhao et al. [35]	2017	Cap	99.0	0.10*	6	293-333	0.1
Domanska et al. [36]	2014	Cap	99.0	0.1	7	323-353	0.1
Moosavi et al. [37]	2013	RBal	99.0	0.5*	3	298-308	0.1
Bajic et al. [38]	2013	RCyl	99.5	0.01	10	288-333	0.1
Bajic et al.[39]	2013	RCyl	99.5	0.01	8	288-323	0.1
Kijevčanin et al.[40]	2013	RCyl	99.5	0.004	8	288-323	0.1
Zarei et al. [41]	2013	Cap	99.5	0.01	6	293-333	0.1
Ling et al. [42]	2011	Cap	na	na	1	298	0.1
Mathuni et al. [43]	2011	Cap	98.0	0.1	1	298	0.1
Doghaei et al. [44]	2010	Cap	99.7	0.01	3	298-308	0.1
Maximino [45]	2009	Cap	99.5	0.003	1	298	0.1
Palani and Geetha [46]	2009	Cap	99.9	na	3	303-313	0.1
Parsa and Faraji [47]	2009	Cap	99.0	na	1	313	0.1
Zarei et al. [48]	2009	Cap	99.5	0.01	1	303	0.1
Nain [49]	2008	Cap	99.3	na	6	293-318	0.1
Parsa and Haghro [50]	2008	Cap	99.0	na	4	293-323	0.1
George and Sastry [51]	2003	Cap	99.5	0.5	5	298-338	0.1
Sastry and Patel [52]	2003	Cap	99.5	0.01	2	298, 308	0.1
Jadzyn et al. [53]	2002	RCyl	99.5	1.0	35	283-363	0.1
Naidu et al. [54]	2002	Cap	Purified	na	1	308	0.1
Kapadi et al. [55]	2001	Cap	Anal.	na	4	303-318	0.1
Saleh et al. [56]	1999	Cap	99.0	na	5	303-323	0.1
Barbetova [57]	1984	Cap	na	0.02	4	283-318	0.1
Idriss-Ali and Freeman [58]	1984	Cap	98.0	na	4	298-358	0.1
Thomas et al. [59]	1979	Cap	Purified	3.0	7	262-338	0.1
Pownall and Smith [60]	1973	Cap	99.0	na	1	296	0.1
Marks [61]	1967	Cap	na	na	1	298	0.1
Timmermans and Hennaut-Roland [62]	1955	na	na	na	2	288, 303	0.1
Kishimoto and Nomoto [63]	1954	Cap	na	na	6	288-313	0.1

<sup>a</sup> Cap, capillary; CC, concentric cylinders; CP, cone and plate; FCyl, falling cylinder; RBal, rolling ball; RCyl, <sup>b</sup> na, not available; Purified, Purified in the laboratory.
 <sup>c</sup> 1 point at atmospheric pressure at the highest temperature of 458 K was not included, as discussed in the text.

\* uncertainty quoted at 95 % confidence level.

There are only two sets of viscosity measurements of propane-1,2-diol performed under high pressures.

- a) The 2017 measurements of Sagdeev et al. [18] were performed in a falling-cylinder viscometer up to 245 MPa and in the temperature range (292 to 458) K, with an uncertainty of 1.5 % to 2 %. Measurements from this group have successfully been employed in previous correlations [6, 7], as well as in the recent reference viscosity correlation of ethane-1,2-diol [9]. However, we do note that in this case, it was impossible to fit the one measurement at atmospheric pressure at the highest temperature of 458 K, which is possibly attributed to high uncertainties in density, as will be discussed at the end of this section. Hence, this single measurement was excluded from the correlation.
- b) The 1988 measurements of Tanaka et al. [24] were also performed in a falling-cylinder viscometer up to 118 MPa pressure in the temperature range (298 to 323) K, with an uncertainty of 2 %. Measurements from this group have also been successfully employed in a previous correlation [6], as well as in the reference correlation of ethane-1,2-diol [9].

Thus, both these sets are included in the primary data set.

As already mentioned in the introduction, propane-1,2-diol is used as a heat transfer liquid, but also extensively employed in experimental studies on volumetric and viscometric properties of binary and ternary mixtures, phase equilibria studies, or even acoustical studies. In such studies, although the viscosity of propane-1,2-diol is also measured, the emphasis is on the properties of the mixture, the solution, and the effect of the change in concentration. Hence, in recent literature there are many papers that include a single measurement of the viscosity of propane-1,2-diol at room temperature with inadequate assessments of uncertainty. As water is the only liquid whose viscosity is known to an uncertainty as low as 0.17 % (at the 95 % confidence level) [10], all measurements in which the authors quote uncertainties of less than 0.1 % (e.g., 0.003 %!), characteristic of investigators that do not understand how to assess their measurement uncertainty, have thus been placed in the secondary data set.

In addition, measurements quoting uncertainties higher than 2 %, and those without any assessment of uncertainty, were placed in the secondary data set. The two measurement sets of the group of Moosavi et al. [32, 37] were also placed in the secondary data because they deviate from the rest of the data by more than the uncertainty quoted by the investigators. Finally, the capillary measurements of George and Sastry [51] and Jadzyn et al. [53] were placed in the secondary data set, as they were 17 and 30 % lower than all other measurements. The remaining sets were kept in the primary data set.



**FIG. 1** Temperature-pressure ranges of the primary experimental viscosity data for propane-1,2-diol. (–) saturation curve



**FIG. 2** Temperature-density ranges of the primary experimental viscosity data for propane-1,2-diol. (–) saturation curve

Figures 1 and 2 show the ranges of the primary measurements outlined in Table 1, and the phase boundary. The primary data are available from the NIST database cited in Ref.[64]. The lack of data in the

vapor phase, near the critical temperature, and in the supercritical region is apparent. The development of the correlation requires densities; Eisenbach et al. [65] has recently developed an accurate, wide-ranging Helmholtz equation of state that is valid from the triple point up to 680 K and 350 MPa. The uncertainties of densities at atmospheric pressure are estimated to be 0.06% at temperatures between 270 and 380 K and increase up to 0.1% at lower temperatures. The uncertainty of calculated densities at elevated pressures is estimated to be 0.06% between 270 and 460 K with pressures up to 100 MPa. Values above 460 K are not fully known due to a lack of high-temperature experimental data. Uncertainties in density in the vapor phase are also not known. We adopt the values for the critical point from their equation of state; the critical temperature,  $T_c$ , and the critical density,  $\rho_c$ , are 674.0 K and 4.46 mol 1<sup>-1</sup>, respectively. We also adopt the value used by Eisenbach et al. [65] for the triple-point temperature, 242.8 K, attributed to Howard [66].

### 2.1 The dilute-gas limit and the initial-density dependence terms

Since there are no measurements in the dilute-gas range we have adopted the procedure employed in the case of the dilute-gas limit viscosity calculation of ethane-1,2-diol [9]. The dilute-gas limit viscosity,  $\eta_0(T)$  is only a function of temperature, can be analyzed independently of all other contributions in Eq. 1, and assuming that the Lennard-Jones potential is applicable, we can employ the Chapman-Enskog theory [67] to express it as

$$\eta_0(T) = 0.02669 \frac{\sqrt{M_{\rm w}T}}{\sigma^2 \Omega^{(2,2)}},\tag{2}$$

where  $M_w$  (g·mol<sup>-1</sup>) is the molar mass,  $\sigma$  is the Lennard-Jones collision diameter in nm, T is the temperature in K, and the resulting viscosity is in µPa·s.  $\Omega^{(2,2)}$  is the Lennard-Jones collision integral that can be calculated by the empirical correlation developed by Neufeld et al. [68] as a function of dimensionless temperature  $T^* = k_{\rm B}T/\varepsilon$  (where  $k_{\rm B}$  is Boltzmann's constant and  $\varepsilon$  is the Lennard-Jones energy parameter),

$$\Omega^{(2,2)}(T^*) = 1.16145(T^*)^{-0.14874} + 0.52487 e^{-0.7732T^*} + 2.16178 e^{-2.43787T^*} - 6.435 \times 10^{-4} (T^*)^{0.14874} \sin\left[18.0323(T^*)^{-0.7683} - 7.27371\right] ,$$
(3)

Since there are no vapor-phase viscosity measurements for propane-1,2-diol available, we employed the empirical equations proposed by Chung et al. [69, 70] to predict the scaling parameters  $\sigma$  (m) and  $\varepsilon/k_{\rm B}$  (K), from

$$\sigma = 8.09 \times 10^{-8} \left( M_{\rm w} / \rho_{\rm c} \right)^{1/3} \qquad \varepsilon / k_{\rm B} = T_{\rm c} / 1.2593 . \tag{4}$$

The resulting values are shown in Table 2. Note that the number of digits given for the critical density are not indicative of the uncertainty, but rather are the result of converting from molar units given in Eisenbach et al.[65] to mass units. Eqs. 2 - 4 present a consistent scheme for the calculation of the dilute-gas limit viscosity of propane-1,2-diol. Figure 3 shows the dilute-gas viscosity as a function of the temperature.

For ease of use in calculations  $\eta_0$  was fit to a polynomial form:

$$\eta_0(T) = \sum_{0}^{4} a_i \left( T / T_c \right)^i,$$
(5)

where the units for  $\eta_0$  are µPa s, *T* is in K, and the coefficients  $\alpha_i$  are in Table 2. Equation 5 reproduces the scheme of Eqs. 2 - 4 to within 0.05 %, and thus it will be employed hereafter. Eq. 5 is easy to implement since it is a simple polynomial, but due to this fact it does not extrapolate well to high temperatures. Any investigative studies that involve behavior above 1500 K should employ the full scheme of Eqs. 2 - 4 which has the correct extrapolation behavior. One also should note that decomposition may need to be considered at elevated temperatures. The equations presented here do not take into account decomposition. Since there are no experimental measurements in the vapor phase, the uncertainty in this region is estimated to be about 15 %. The application of the technique to other compounds where vapor-phase measurements exist, e.g., *n*-hexane [8] and *n*-heptane [7], have demonstrated an uncertainty of 10%; however due to the polar nature of propane-1,2-diol the uncertainty of the method may be slightly higher.



FIG. 3 Dilute-gas viscosity as a function of the temperature, calculated by the scheme of Eqs. (2)-(4)

The temperature dependence of the linear-in-density coefficient of the viscosity,  $\eta_1(T)$ , in Eq. 1 is large at temperatures below critical and must be considered to obtain an accurate representation of the behavior of the viscosity in the vapor phase. In addition,  $\eta_1(T)$  changes sign from positive to negative as the temperature decreases. Therefore, the viscosity along an isotherm should first decrease in the vapor phase and subsequently increase with increasing density [71, 72]. Vogel et al. [72] have shown that fluids exhibit the same general behavior of the initial density dependence of viscosity, which can also be expressed by means of the second viscosity virial coefficient  $B_\eta(T)$  in m<sup>3</sup> kg<sup>-1</sup>, as

$$B_{\eta}(T) = \frac{\eta_1(T)}{\eta_0(T)}.$$
 (6)

Note that in the above equation, if the dilute-gas limit viscosity,  $\eta_0(T)$ , is expressed in  $\mu$ Pa s, then the initialdensity viscosity coefficient,  $\eta_1(T)$ , will be expressed in  $\mu$ Pa s m<sup>3</sup> kg<sup>-1</sup>. The second viscosity virial coefficient can be obtained according to the theory of Rainwater and Friend [11, 12] as a function of a reduced second viscosity virial coefficient,  $B_{\eta}^{*}(T^{*})$ , as

$$B_{\eta}^{*}(T^{*}) = \frac{B_{\eta}(T)M_{W}}{N_{A}\sigma^{3}},$$
(7)

where [72]

$$B_{\eta}^{*}(T^{*}) = \sum_{i=0}^{6} b_{i} \left(T^{*}\right)^{-0.25i} + b_{7} \left(T^{*}\right)^{-2.5} + b_{8} \left(T^{*}\right)^{-5.5}.$$
(8)

In Eq. 7,  $N_A$  is the Avogadro constant and  $T^*$  as defined earlier. The coefficients  $b_i$  from Ref. [72] are given in Table 2. Figure 4 shows the calculated values of the initial-density viscosity coefficient, employing the scheme described by Eqs. 5 - 8.

Table 2	Coefficients	and	parameters	for	Eqs.	2 ·	- 8
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$\varepsilon/k_{\rm B}$ (K)	535.2
$\sigma$ (nm)	0.4915
$M_{\rm w}$ (g mol <sup>-1</sup> )	76.09442
$T_{\rm c}({\rm K})$	674.0
$ ho_{\rm c}$ (kg m <sup>-3</sup> )	339.3811132
Coefficients $a_i$ (µPa	s) for Eq. 5
0	1.15331
1	$1.06228 \times 10^{1}$
2	$1.31421 \times 10^{1}$
3	-9.37974
4	2.08103
Coefficients $b_i$ (-) for	r Eq. 8 [72]
0	-1.9572881×101
1	2.1973999×10 <sup>2</sup>
2	-1.0153226×10 <sup>3</sup>
3	2.4710125×10 <sup>3</sup>
4	-3.3751717×10 <sup>3</sup>
5	2.4916597×10 <sup>3</sup>
6	-7.8726086×10 <sup>2</sup>
7	1.4085455×10 <sup>1</sup>
8	-3.4664158×10 <sup>-1</sup>



**FIG. 4** Initial-density viscosity coefficient  $\eta_1$  calculated from the scheme of Eqs. (5)-(8)

# 2.2 The residual term

As stated in Section 2, the residual viscosity term,  $\Delta \eta(\rho, T)$ , represents the contribution of all other effects to the viscosity of the fluid at elevated densities, including many-body collisions, molecular-velocity correlations, and collisional transfer. As there is no rigorous theory to calculate this term, it was evaluated almost entirely on experimentally obtained data, as discussed in the next paragraph.

The procedure adopted during this analysis used symbolic regression software [73] to fit all the primary data to the residual viscosity. Symbolic regression is a type of genetic programming that allows the exploration of arbitrary functional forms to regress data. The functional form is obtained by use of a set of operators, parameters, and variables as building blocks. Most recently this method has been used to obtain correlations for the viscosity of ethane-1,2-diol [9], R161 [1], *n*-undecane [2], R1234yf and R1234ze(E) [5], ammonia [74], and xenon [75]. In the present work, we restricted the operators to the set (+,-,\*,/) and the operands (constant,  $T_r$ ,  $\rho_r$ ), with  $T_r = T/T_c$  and  $\rho_r = \rho/\rho_c$ . As mentioned earlier, the critical temperature  $T_c = 674.0$  K and critical density  $\rho_c = 4.46$  mol 1<sup>-1</sup> are from the equation of state of Eisenbach et al. [65]. In

addition, we adopted a form suggested by the hard-sphere model employed by Assael et al. [76],  $\Delta \eta(\rho_r, T_r) = (\rho_r^{2/3} T_r^{1/2}) F(\rho_r, T_r)$ , where the symbolic regression method was used to determine the functional form for  $F(\rho_r, T_r)$ . For this task, the dilute-gas limit and the initial density dependence term were calculated for each experimental point, employing Eqs. 5 - 8, and subtracted from the experimental viscosity to obtain the residual term,  $\Delta \eta(\rho_r, T_r)$ . The objective function was the natural logarithm of the difference between the experimental and calculated values of the residual term, and data were weighted equally. The density values employed were obtained by the equation of state of Eisenbach et al. [65]. The final equation obtained was

$$\Delta\eta(\rho,T) = \eta_{\rm ref}(\rho_{\rm r}^{2/3}T_{\rm r}^{1/2})\exp\left\{c_0 + c_1\rho_{\rm r} + \frac{c_2\rho_{\rm r}^2}{T_{\rm r}} + c_3\frac{\rho_{\rm r}^3}{T_{\rm r}^2} + c_4T_{\rm r} + c_5T_{\rm r}^2\right\}$$
(9)

Coefficients  $c_i$  are given in Table 3, and  $\Delta \eta$  is in  $\mu$ Pa s.

**Table 3** Coefficients  $c_i$  for Eq. 9

$c_0$	6.17070938	
$c_1$	3.15366627	
$c_2$	-6.87686250×10 <sup>-1</sup>	
<i>c</i> <sub>3</sub>	8.79750441×10 <sup>-2</sup>	
<i>C</i> 4	$-1.02553117 \times 10^{1}$	
C5	4.36659437	
η <sub>ref</sub> (μPa s)	1.0	

#### 2.3 Comparison with data

Tables 4 and 5 summarize comparisons of the primary and secondary data with the correlation. We have defined the percent, or relative deviation as PCTDEV =  $100(\eta_{exp}-\eta_{fit})/\eta_{fit}$ , where  $\eta_{exp}$  is the experimental value of the viscosity and  $\eta_{fit}$  is the value calculated from the correlation. Thus, the average absolute relative deviation (AAD) is found with the expression AAD = ( $\sum |PCTDEV|$ )/*n*, where the summation is over all *n* points, the bias is found with the expression BIAS = ( $\sum PCTDEV$ )/*n*. The average absolute relative deviation of the fit for all primary data is 1.68 %, with a bias of -0.3 %. At the 95% confidence level (*k* = 2), the relative uncertainty of the correlation from the triple point up to 452 K and 245 MPa is 4.5 %. For regions where there were no data available for comparison the deviations may be higher.

Investigators / Reference	AAD (%)	BIAS (%)
Azarang et al. [16]	0.74	0.12
Miksik et al. [17]	1.47	-0.59
Sagdeev et al. [18]	2.32	-1.07
Soldatovic et al. [19]	0.54	0.54
Zivkovic et al. [20]	1.46	0.29
Zivkovic et al. [21]	0.64	-0.29
Tsai et al. [22]	2.11	-2.11
Sun and Teja [23]	1.50	1.23
Tanaka et al. [24]	0.61	0.61
Vinogradov and Shakhparonov [25]	2.32	0.41
Litovitz et al. [26]	4.28	4.28
Entire set	1.68	-0.3

Table 4 Evaluation of propane-1,2-diol viscosity correlation for the primary data

Figure 5 shows the relative deviations of all primary viscosity data of propane-1,2-diol from the values calculated by Eqs. 1, 5 - 9, as a function of temperature, while Figs. 6 and 7 show the same deviations but as a function of the pressure and the density. The deviations of the experimental data from the present correlation are within about 4.5 %. This fluid would benefit from additional measurements. There are also no vapor-phase measurements at all. The availability of vapor-phase measurements would assist in better understanding of the gas-phase behavior of glycols.

Figure 8 shows the viscosity as a function of temperature along selected isobars, while Table 5 presents the deviations of the secondary data from the proposed correlation.



**FIG. 5** Relative deviations of primary experimental data of propane-1,2-diol from the values calculated by the present model as a function of temperature. Azarang et al. [16] ( $\diamond$ ), Miksik et al. [17] ( $\blacklozenge$ ), Sagdeev et al. [18] ( $\blacklozenge$ ), Soldatovic et al. [19] (⊕), Zivkovic et al. [20] ( $\blacksquare$ ), Zivkovic et al. [21] ( $\blacksquare$ ), Tsai et al. [22] (⊕), Sun and Teja [23] ( $\Box$ ), Tanaka et al. [24] ( $\bigcirc$ ), Vinogradov and Shakhparonov [25] ( $\blacksquare$ ), Litovitz et al. [26] ( $\blacktriangle$ )



FIG. 6 Relative deviations of primary experimental data of propane-1,2-diol from the values calculated by the present model as a function of pressure. Azarang et al. [16] (◇), Miksik et al. [17] (◆), Sagdeev et al. [18] (●), Soldatovic et al. [19] (□), Zivkovic et al. [20] (□), Zivkovic et al. [21] (□), Tsai et al. [22] (
(●), Sun and Teja [23] (□), Tanaka et al. [24] (○), Vinogradov and Shakhparonov [25] (■), Litovitz et al. [26] (▲)



FIG. 7 Relative deviations of primary experimental data of propane-1,2-diol from the values calculated by the present model as a function of density. Azarang et al. [16] (◊), Miksik et al. [17] (♦), Sagdeev et al. [18] (●), Soldatovic et al. [19] (Φ), Zivkovic et al. [20] (■), Zivkovic et al. [21] (□), Tsai et al. [22] (
(●), Sun and Teja [23] (□), Tanaka et al. [24] (○), Vinogradov and Shakhparonov [25] (■), Litovitz et al. [26] (▲).



FIG. 8 Viscosity of propane-1,2-diol as a function of the temperature for different pressures

Investigators/ Reference	AAD (%)	BIAS (%)
Hema et al. [27]	9.73	-9.73
Trenzado et al.[28]	1.33	0.55
Akilu et al. [29]	2.71	-2.38
Esteban and Gonzalez-Miquel [30]	3.21	3.21
Yang et al. [31]	1.06	-0.27
Moosavi et al. [32]	3.87	-2.11
Cano-Gomez et al. [33]	0.60	0.53
Khattab et al. [34]	15.70	-15.70
Domanska et al. [36]	5.70	-3.86
Moosavi et al. [37]	1.28	0.76
Bajic et al. [38]	1.65	1.65
Bajic et al. [39]	0.92	0.92
Kijevčanin et al.[40]	0.64	-0.28
Zarei et al. [41]	1.64	0.27
Ling et al. [42]	0.64	0.64
Mathuni et al. [43]	1.50	1.50
Doghaei et al. [44]	3.86	3.86
Maximino [45]	0.78	0.78
Palani and Geetha [46]	46.10	-46.10
Parsa and Faraji [47]	0.85	-0.85
Zarei et al. [48]	2.87	2.87
Nain [49]	9.04	0.52
Parsa and Haghro [50]	2.34	-0.92
George and Sastry [51]	5.61	-4.91
Sastry and Patel [52]	2.27	-2.27
Jadzyn et al. [53]	21.84	-21.84
Naidu et al. [54]	0.61	0.61
Kapadi et al. [55]	1.21	0.34
Saleh et al. [56]	4.02	-4.02
Barbetova [57]	4.33	-4.33
Idriss-Ali and Freeman [58]	2.75	2.75
Thomas et al. [59]	3.76	0.88
Pownall and Smith [60]	2.11	-2.11
Marks [61]	1.25	-1.25
Timmermans and Hennaut-Roland [62]	46.94	46.94
Kishimoto and Nomoto [63]	61.79	61.79

**Table 5** Evaluation of propane-1,2-diol viscosity correlation for the secondary data.

#### **3** Recommended Values

In Table 6, viscosity values are given along the saturated liquid and vapor curves, calculated from the present proposed correlations between 245 and 450 K, while in Table 7 viscosity values are given for temperatures between 245 and 450 K at selected pressures. Saturation pressure and saturation density values for selected temperatures, as well as the density values for the selected temperature and pressure, are obtained from the equation of state of Eisenbach et al. [65]. The calculations are performed at the given temperatures and densities. For computer verification of values, the following points may be used for the given *T*,  $\rho$  conditions: T = 350 K,  $\rho = 0.0$  kg m<sup>-3</sup>,  $\eta = 9.051368$  µPa s; T = 350 K,  $\rho = 0.02$  kg m<sup>-3</sup>,  $\eta = 9.058162$  µPa s; T = 350 K,  $\rho = 1000.0$  kg m<sup>-3</sup>,  $\eta = 5135.986461$  µPa s.

Т (К)	p (MPa)	$ ho_{ m liq}$ (kg m <sup>-3</sup> )	$ ho_{ m vap}$ (kg m <sup>-3</sup> )	η <sub>liq</sub> (μPa s)	η <sub>vap</sub> (μPa s)
245	4.4336×10 <sup>-8</sup>	1072.3	1.6562×10 <sup>-6</sup>	4683847.	6.34
270	1.0456×10 <sup>-6</sup>	1053.7	3.5441×10 <sup>-5</sup>	331522.	6.97
290	8.3332×10 <sup>-6</sup>	1038.7	2.6299×10 <sup>-4</sup>	72640.	7.48
310	4.8554×10-5	1023.5	1.4335×10 <sup>-3</sup>	22922.	8.00
330	2.1980×10 <sup>-4</sup>	1007.9	6.0969×10 <sup>-3</sup>	9387.5	8.53
350	8.0999×10 <sup>-4</sup>	991.96	2.1190×10 <sup>-2</sup>	4662.3	9.06
370	2.5195×10 <sup>-3</sup>	975.55	6.2392×10 <sup>-2</sup>	2671.0	9.59
390	6.8069×10 <sup>-3</sup>	958.6	1.6014×10 <sup>-1</sup>	1704.5	10.13
410	1.6343×10 <sup>-2</sup>	941.01	3.6665×10 <sup>-1</sup>	1180.9	10.67
430	3.5521×10 <sup>-2</sup>	922.68	7.6302×10 <sup>-1</sup>	871.26	11.22
450	7.0961×10 <sup>-2</sup>	903.48	1.4659	674.54	11.76

 Table 6
 Viscosity values of propane-1,2-diol along the saturation curve, calculated by the present scheme

p (MPa)	Т (К)	ρ (kg m <sup>-3</sup> )	η (μPa s)	p (MPa)	Т (К)	ho (kg m <sup>-3</sup> )	η (μPa s)
0.1	245	1072.3	4683847.	150	300	1089.2	124184.
	270	1053.7	331522.		330	1071.2	24422.
	300	1031.2	39323.		360	1053.2	7911.9
	330	1008.0	9407.		390	1035.2	3551.2
	360	983.89	3477.7		420	1017.0	1982.8
	390	958.67	1705.6		450	998.75	1289.5
	420	932.02	1007.9				
	450	903.51	674.67				
50	245	1091.6	9060255.	240	335	1095.4	30348.
	270	1074.4	566087.		360	1081.8	11508.
	300	1053.8	60475.		390	1065.6	4901.9
	330	1033.1	13523.		420	1049.5	2639.8
	360	1012.0	4786.4		450	1033.4	1672.3
	390	990.36	2281.5				
	420	968.12	1327.8				
	450	945.09	885.40				
100	270	1091.9	907832.				
	300	1072.7	88176.				
	330	1053.6	18475.				
	360	1034.3	6249.8				
	390	1014.8	2890.2				
	420	995.03	1648.8				
	450	974.86	1086.7				

**Table 7** Viscosity values of propane-1,2-diol at selected temperatures and pressures, calculated by the present scheme. Values are computed at the given temperatures and densities

# 4 Conclusions

A new wide-ranging correlation for the viscosity of propane-1,2-diol was developed based on critically evaluated experimental data and theoretical results. The dilute-gas limit viscosity in the present work was calculated from the Chapman-Enskog theory [67], by employing the empirical equations of Neufeld et al. [68] and Chung et al. [69, 70], and then fit to a polynomial for convenience. The initial-density dependence viscosity is based on the scheme proposed by Vogel et al. [72], and the residual term is based on a critically evaluated set of measurements. Due to the lack of experimental data in the vapor phase, the uncertainty in

the dilute-gas region is estimated to be approximately 15 %, while in all other cases it is 4.5 % (at the 95% confidence level). Since we could not locate any gas-phase measurements, we recommend experimental measurements be made to assist in the understanding of the vapor-phase behavior of glycols. The correlation is valid for temperatures from the triple-point temperature to 452 K and for pressures up to 245 MPa. Both limits are imposed by the range of the primary experimental data. Although there are multiple data sets at atmospheric pressure, many of these disagree by more than their uncertainties; additional measurements in these regions, and at pressures above atmospheric, would be helpful for the development of an improved correlation. The correlation behaves in a physically realistic manner at temperatures and pressures up to 680 K and 350 MPa, respectively, and we feel the correlation may be extrapolated to this limit, although the uncertainty will be larger, decomposition may need to be considered, and caution is advised.

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