

## Boyle temperatures for pure substances

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### Abstract

We report Boyle temperatures of 83 pure substances calculated using the Zeno (unit compressibility) line from standard or reference equations of state (EOS). We compare the results using different EOS and from correlations already published in the literature. The maximum absolute difference in the calculation of the Boyle temperature from different EOS is 15, 3, 24 and 63 K for hydrocarbons, gases, freons, and other substances, respectively. For alcohols, the difference in calculated Boyle temperatures is 300 K for methanol and 5 K for ethanol.

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### 1. Introduction

The Boyle temperature is the temperature at which the second virial coefficient becomes zero, and it is a useful reducing parameter in some cases. However, because Boyle temperatures are usually relatively high, their determination is rather difficult experimentally. The Boyle temperature is also the extrapolation to zero density of a collection of temperature–density values for which the compressibility factor is unity. Several authors have used this latter approach to calculate the Zeno line and find the Boyle temperature. Batschinski [1] discovered this extrapolation first and later several authors [2–4] rediscovered it. Holleran et al. [5] have used the Zeno line and the Boyle temperature to correlate critical points, compressed liquid densities [6], EOS for liquids [7], and general EOS studies [8]. Xu and Herschbach [9] correlate the Zeno line and critical properties using the Boyle temperature as a reducing parameter. Recently, Iglesias-Silva and Hall [10] use the Boyle temperature to correlate the second virial coefficients of non-polar and polar substances with single temperature functionality.

In this work, we use the standard or reference EOS from the literature to calculate the Boyle temperatures of pure non-

polar and polar substances. It has been a common practice to calculate the Boyle temperature for the most common non-polar substances using different EOS.

### 2. Calculation of the Boyle temperature

The Boyle temperature is the temperature at which the second virial coefficient becomes zero for a given substance. When the compressibility factor equals unity, the virial EOS reduces to

$$0 = B + C\rho + D\rho^2 + E\rho^3 + \dots \quad (1)$$

Thus, at zero density, when the compressibility factor is unity, the second virial coefficient is zero and the corresponding temperature is the Boyle temperature. Plotting the values of temperature versus density when the compressibility factor equals unity, the intercept corresponds to the Boyle temperature. We use this procedure to find the Boyle temperature of pure substances in this paper.

### 3. Standard or reference equation of state

A standard or reference EOS is a multi-parametric equation with a high level of accuracy required for scientific and technical applications. These EOS are developed by optimizing a functional form based upon the most complete data set existing

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in the literature of PVT, virial coefficients, heat capacities, enthalpy, speed of sound, Joule–Thompson coefficient, and any other available measurements. The functional form generally consists of high degree polynomials in temperature and density with exponential functions, and their performance is better than physically based EOS. These EOS should have a good extrapolation behavior [11], but an extensive study has not confirmed this assumption. Recently, Span and Wagner [12,13] and Sun and Ely [14] have attempted to homogenize the number of functional terms for several substances without losing accuracy in representing the data set that they used to optimize the parameters. Most of the reference EOS belongs to the group of modified Benedict-Webb-Rubin equations formulated in the Helmholtz energy:

$$\begin{aligned} \frac{A(T, \rho)}{RT} &= \alpha^\circ(\tau, \delta) + \alpha^r(\tau, \delta) \\ &= \alpha^\circ(\tau, \delta) + \sum_{i=1}^{N_1} n_i \tau^{t_i} \delta^{d_i} + \sum_{i=N_1+1}^{N_1+N_2} n_i \tau^{t_i} \delta^{d_i} \exp(-\delta^{p_i}) \end{aligned} \quad (2)$$

where  $A$  is the molar Helmholtz energy,  $\alpha^\circ$  and  $\alpha^r$  are the ideal gas and residual part of the Helmholtz energy,  $R$  the universal gas constant,  $T$  the temperature,  $\rho$  the density,  $\tau$  the dimensionless temperature equal to  $T_c/T$ , and  $\delta$  is dimensionless density equal to  $\rho/\rho_c$ .  $N_1$  and  $N_2$  are the number of polynomial and polynomial plus exponential terms and  $n_i$ ,  $t_i$ ,  $d_i$  and  $p_i$  are the adjusted parameters selected from a data bank of hundreds of terms. The compressibility factor from Eq. (2) is

$$\begin{aligned} Z &= \frac{P}{\rho RT} \\ &= 1 + \delta \left( \frac{\partial \alpha^r}{\partial \delta} \right)_\tau \\ &= 1 + \sum_{i=1}^{N_1} n_i d_i \tau^{t_i} \delta^{d_i} + \sum_{i=N_1+1}^{N_1+N_2} n_i \tau^{t_i} \delta^{d_i} (d_i - p_i \delta^{p_i}) \exp(-\delta^{p_i}) \end{aligned} \quad (3)$$

For unit compressibility, Eq (3) becomes

$$\sum_{i=1}^{N_1} n_i d_i \tau^{t_i} \delta^{d_i} + \sum_{i=N_1+1}^{N_1+N_2} n_i \tau^{t_i} \delta^{d_i} (d_i - p_i \delta^{p_i}) \exp(-\delta^{p_i}) = 0 \quad (4)$$

With reference equations of this type, we use Eq. (4) to calculate the density at a given temperature. Table 1 contains the sources of the different EOS considered in this work.

#### 4. Results and discussion

We have calculated the Boyle temperature of non-polar and polar pure substances using reference EOS shown in Table 1. Values of the Boyle temperatures and sources of the EOS also appear in Table 1. We have used a correlation developed by Hall and Iglesias-Silva [10] and compare it to our results. The behavior appears in Fig. 1, and the average percentage deviation of this correlation with respect to the Boyle temperatures is 3.5%.

Table 1  
Boyle temperatures of pure substances

Substance	$T_C$ (K)	$T_{Boyle}$ (K)	Source
Hydrocarbons			
Methane	190.56	509.74	[28]
		509.07	[12]
		513.14	[14]
Ethane	305.33	768.49	[29]
		769.84	[12]
		772.25	[14]
Ethylene	282.35	724.33	[30]
		723.27	[12]
		724.63	[14]
		722.39	[31]
Propane	369.83	902.56	[32]
		903.8	[12]
		912.19	[14]
		903.34	[33]
Propylene	365.57	886.38	[34]
Propyne	402.38	942.10	[35]
Butane	425.13	1017.70	[36]
		1019.2	[12]
		1031.3	[14]
		1034.4	[33]
1-Butene	419.29	1008.30	[37]
Isobutane	407.82	984.54	[38]
		984.53	[12]
		992.14	[14]
		978.16	[33]
Isobutene	418.09	1013.60	[37]
<i>trans</i> -Butene	428.61	1039.80	[37]
<i>cis</i> -2-Butene	435.75	1049.40	[37]
Pentane	469.70	1113.50	[39]
		1113.1	[12]
		1110.4	[14]
		1130.4	[15]
Isopentane	460.35	1107.20	[40]
		1101.50	[15]
Neopentane	433.74	1029.10	[40]
Cyclopentane	398.30	975.72	[35]
Hexane	507.82	1185.50	[39]
		1185.6	[12]
		1174	[14]
		1152.7	[15]
Isohexane	497.70	1171.60	[40]
Cyclohexane	553.64	1314.40	[41]
		1302.5	[12]
		1306.5	[14]
Heptane	540.13	1252.30	[39]
		1246	[12]
		1279	[15]
Octane	569.32	1311.60	[37]
		1300.6	[12]
		1296.1	[14]
		1784.3	[15]
Nonane	594.55	1339.40	[40]
Decane	617.70	1370.20	[40]
Dodecane	658.10	1403.10	[42]

Table 1 (Continued)

Substance	$T_C$ (K)	$T_{Boyle}$ (K)	Source
Gases			
Argon	150.69	407.76	[43]
		407.59	[12]
		408.35	[44]
Carbon monoxide	304.13	341.32	[40]
Carbon dioxide	132.86	717.93	[45]
		716.68	[13]
		719.00	[14]
Deuterium	38.34	113.70	[46]
Helium	5.20	22.58	[47]
Hydrogen	33.19	109.43	[48]
		106.96	[49]
Krypton	209.48	569.61	[40]
		566.80	[50]
Neon	44.49	120.32	[51]
Nitrogen	126.19	326.41	[52]
		325.77	[12]
		328.37	[14]
		325.41	[53]
Nitrous oxide	309.58	754.80	[40]
Oxygen	154.58	408.35	[54]
		411.46	[12]
Parahydrogen	32.94	110.51	[48]
Sulfur dioxide	430.64	1042.70	[40]
Xenon	289.73	792.81	[40]
		795.62	[55]
Alcohols			
Methanol	512.60	1439.20	[56]
		1094.7	[14]
Ethanol	513.93	1283.90	[57]
		1281.4	[14]
1-Propanol	536.7	1435.6	[14]
Freons			
R11	471.11	1151.10	[58]
		1133.3	[13]
R113	487.21	1145.20	[59]
		1144.1	[13]
R114	418.83	968.19	[60]
R115	353.10	792.12	[61]
R116	293.03	667.71	[40]
R12	385.12	929.69	[59]
		934.09	[13]
		926.39	[62]
R123	456.83	1058.40	[63]
		1068.6	[13]
		1065.3	[64]
R124	395.43	926.63	[65]
R125	339.17	770.76	[66]
		772.85	[13]
		770.96	[14]
		763.33	[67]

Table 1 (Continued)

Substance	$T_C$ (K)	$T_{Boyle}$ (K)	Source
R13	302.00	733.97	[68]
R134a	374.21	875.33	[69]
		868.34	[13]
		866.67	[14]
R14	227.51	528.80	[60]
R141b	477.50	1141.20	[40]
R142b	410.26	982.17	[40]
R143a	345.86	828.70	[70]
		833.59	[13]
R152a	386.41	938.69	[71]
		940.73	[13]
R21	451.48	1086.20	[60]
R218	345.02	790.37	[38]
R22	369.30	888.29	[72]
		889.19	[13]
R227ea	375.95	852.28	[40]
R23	299.29	717.29	[73]
		693.06	[60]
R236ea	412.44	923.03	[61]
R236fa	398.07	898.17	[74]
R245ca	447.57	1060.40	[61]
R245fa	427.20	977.95	[61]
R32	351.26	865.67	[75]
		859.24	[13]
		867.36	[14]
R41	317.28	818.81	[40]
RC318	388.38	827.02	[60]
Others			
Sulfur hexafluoride	318.73	727.48	[76]
		738.4	[12]
Toluene	591.75	1403.10	[40]
		1401.5	[14]
Water	647.10	1599.60	[77]
		1662.6	[14]
Acetone	508.10	1238.80	[40]
Ammonia	405.40	1034.20	[78]
		1033.7	[13]
		1024.3	[14]
Benzene	562.05	1326.50	[35]
		1340.3	[14]
Decafluorobutane	386.33	913.39	[53]
Dodecafluorobutane	420.56	902.31	[53]
Carbonyl sulfide	378.77	967.76	[38]
Dimethylether	400.10	991.85	[61]
Fluorine	144.41	383.62	[79]
Hydrogen sulfide	373.10	942.63	[40]
		804.82	[15]
Nitrogen trifluoride	234.00	568.46	[44]

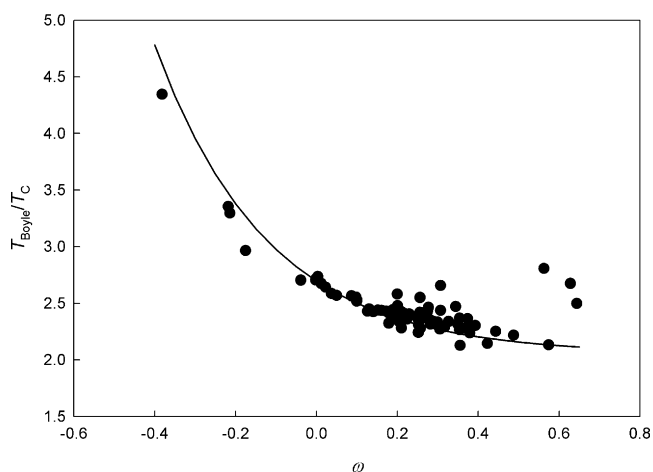


Fig. 1. Comparison between Iglesias-Silva and Hall correlation (—), and the Boyle temperatures (●), obtained in this work.

Recently, Span and Wagner [12,13] and Sun and Ely [14] have developed modified BWR EOS. The former authors develop two general functional forms for non-polar and polar substances while the latter authors present a single general functional form for non-polar and polar substances including normal alcohols. These equations have fewer characteristic constants (up to 15) than reference EOS. We have used these equations also to calculate the Boyle temperature and the results appear in Table 1. The EOS developed by Starling [15] predicts, for some substances, Boyle temperatures different than the rest of the EOS. This is an indication of that it does not have good extrapolation capabilities. Without considering this work, the maximum absolute difference when we compare the results from different EOS is 15, 3, 24 and 63 K for hydrocarbons, gases, freons, and other substances, respectively. For alcohols, there are only two different EOS and the agreement in the calculated Boyle temperatures is 300 K for methanol and 5 K for ethanol, as shown in Table 1.

Also, we have found that an anomalous Zeno line exists that lies within the equilibrium dome for modified BWR EOS. Fig. 2 shows the Zeno line, the saturation curve, and the anomalous Zeno line for methane. For the anomalous line to be true, it

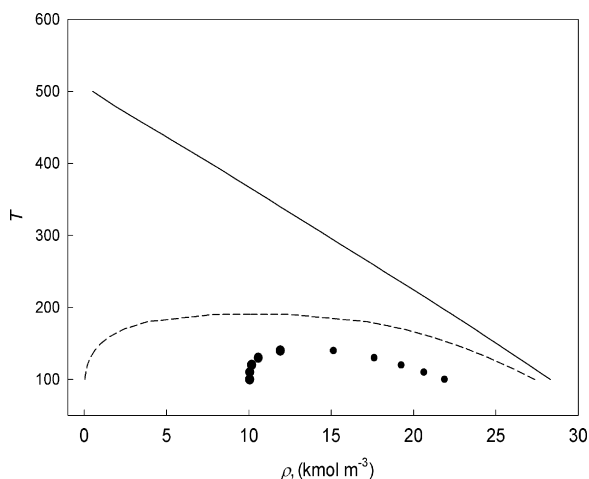


Fig. 2. Zeno line (—), the saturation curve (---), and anomalous Zeno line (●) for methane.

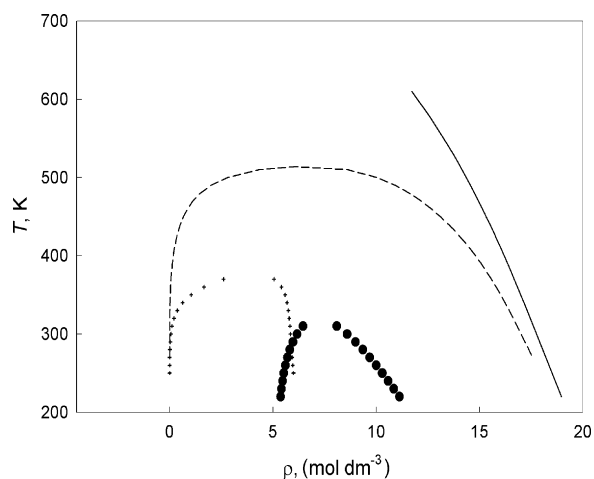


Fig. 3. Zeno line (—), the saturation curve (---), and two different anomalous Zeno lines from different EOS for ethanol (●), Sun and Ely [14]; Dillon and Penoncello [15] (■).

would need to have  $Z^V > 1$  and  $Z^L < 1$ . The non-linear and high degree polynomials make these EOS exhibit this unnecessary root. In some cases, for example ethanol, two reference BWR equations [14,16] can have two different spurious Zeno lines as shown in Fig. 3. However, this behavior is not present in cubic EOS. For example, the van der Waals (vdW), Redlich-Kwong (RK), Soave-Redlich-Kwong (SRK) EOS have the trivial root ( $\rho_R = 0$ ) and one real root, while the Peng-Robinson equation of state has two real roots. The first real root gives unreasonable values of the reduced density that lie outside the equilibrium dome. Powles [17] and Heyes and Llaguno [18] have calculated expressions for the Boyle temperature from cubic EOS. Fig. 4 shows the reduced temperature behavior as a function of the reduced density for *n*-pentane from different EOS. Although the only EOS with linear behavior is the vdW, some of the values lie inside the equilibrium dome, as shown in Fig. 4. The influence of the acentric factor in the calculation of the temperature–density behavior using the SRK starts after a reduced temperature of unity where all the curves intercept, as shown in Fig. 5. Recently,

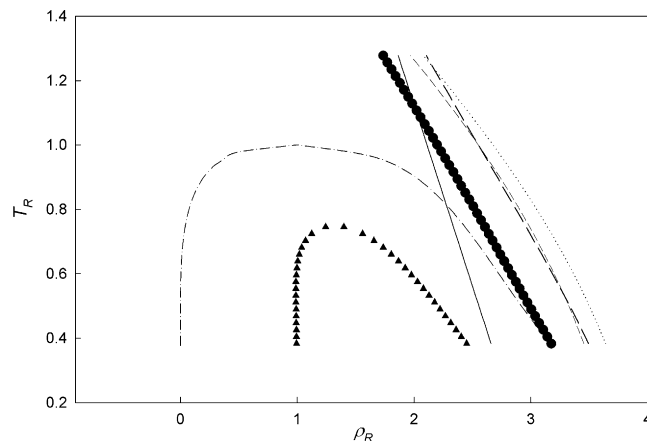


Fig. 4. Reduced temperature behavior as a function of the reduced density for *n*-pentane from cubic EOS when  $Z = 1$ : (●) Zeno line; (▲) anomalous Zeno line; (---) saturation curve; (—) vdW; (---) RK; (···) SRK; (-·-) PR.

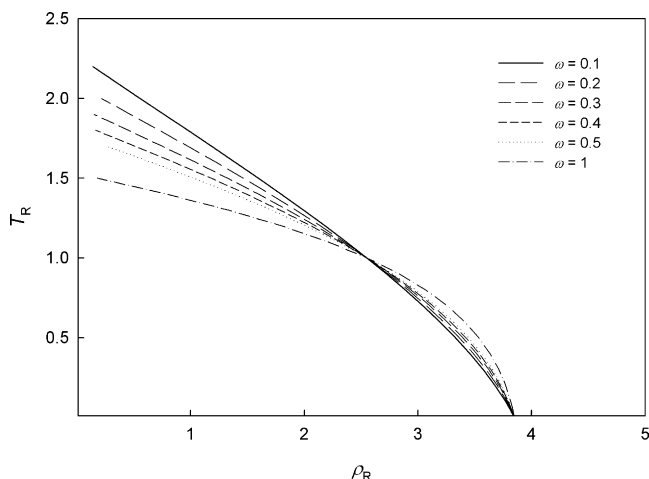


Fig. 5. Reduced temperature behavior as a function of the reduced density for different acentric factors.

Kutney et al. [19] show various contours of the compressibility factor including  $Z = 1$  using the PR and SRK for water, methane and carbon dioxide. Also, they compare the Zeno line of water from these equations with the results obtained from molecular dynamics simulations.

We have compared our results for hydrocarbons with those obtained from molecular simulations by Vega and López-Rodríguez [20]. They calculate the Boyle temperature of  $n$ -alkanes with up to 200 carbon atoms. It is clear that the Boyle temperature does not exist physically for these high molecular weight molecules, but because this temperature is a reference point, their results can provide estimates for high molecular weight  $n$ -alkanes. We have represented the Boyle temperature of these substances as

$$T_{\text{Boyle}} = 57.8 + \frac{1646.222n}{2.7 + n} \quad (5)$$

where  $n$  is the number of carbon atoms. Fig. 6 shows the behavior of Eq. (5).

We can observe that when the virial data cross zero, determination of the Boyle temperature is equivalent if one uses the

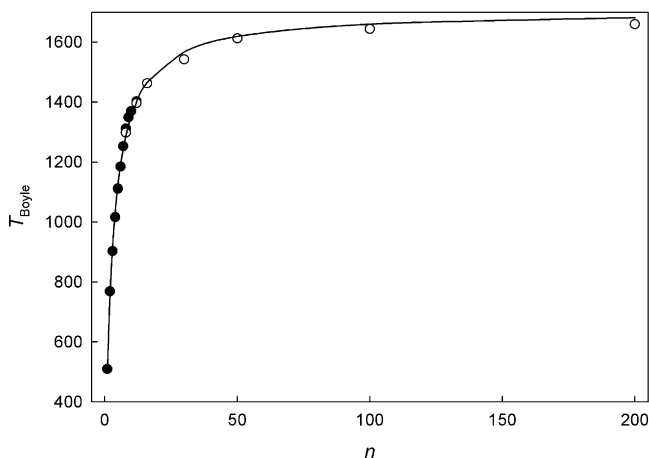


Fig. 6. Boyle temperature for  $n$ -alkanes as a function of the carbon number: (—) Eq. (5); (●) this work; (○) Vega and López-Rodríguez [19].

Table 2

Boyle temperatures from the Tsionopoulos correlation [22,23], a modification of the Tsionopoulos correlation [24], and a correlation based upon square-well potential [25]

Substance	$T_{\text{Boyle}}$ (K) [22,23]	$T_{\text{Boyle}}$ (K) [24]	$T_{\text{Boyle}}$ (K) [25]
<b>Hydrocarbons</b>			
Methane	503.15	510.19	508.35
Ethane	770.06	757.36	778.00
Ethylene	716.03	706.55	745.64
Propane	907.92	879.76	943.23
Propylene	902.72	877.39	934.47
Propyne	962.81	921.59	
Butane	1019.25	976.47	1053.55
1-Butene	1009.23	968.60	1006.48
Isobutane	985.03	946.89	967.48
Isobutene	1005.84	965.13	
<i>trans</i> -Butene	1022.56	977.51	1095.56
<i>cis</i> -2-Butene	1043.69	999.44	997.2
Pentane	1098.47	1041.53	1195.91
Isopentane	1087.81	1035.69	1200.85
Neopentane	1041.95	999.11	1098.96
Cyclopropane	988.68	963.63	
Hexane	1160.75	1091.61	1266.63
Isohexane	1147.90	1082.84	
Cyclohexane	1321.33	1263.32	1426.13
Heptane	1206.18	1126.29	1319.72
Octane	1246.15	1157.61	1377.33
Nonane	1272.79	1176.70	
Decane	1296.83	1194.83	
Dodecane	1332.98	1222.59	
<b>Gases</b>			
Argon	400.76	408.61	409.14
Carbon monoxide	343.75	343.58	342.01
Carbon dioxide	720.65	686.90	712.17
Deuterium	112.11	125.35	
Helium	17.16	23.43	
Hydrogen	99.23	114.11	108.47
Krypton	556.73	567.33	571.19
Neon	120.66	124.98	122.54
Nitrogen	328.69	330.04	325.11
Nitrous oxide	756.74	731.67	791.73
Oxygen	405.83	409.79	398.69
Parahydrogen	98.70	113.86	
Sulfur dioxide	1005.60	951.93	1053.93
Xenon	768.16	781.34	
<b>Alcohols</b>			
Methanol	1038.22		1056.84
Ethanol	1007.04		917.12
1-Propanol	1059.43		
<b>Freons</b>			
R11	1135.78	1090.65	
R113	1138.58		
R114	978.89	927.83	
R115	825.38	782.01	
R116	683.32		
R12	932.75	897.75	
R123	1052.68	992.74	
R124	908.53	855.92	
R125	773.02	726.23	
R13	734.05	707.57	
R134a	844.44	790.99	
R14	551.29	530.76	
R141b	1133.66	1081.47	
R142b	968.42	921.64	

Table 2 (Continued)

Substance	$T_{\text{Boyle}}$ (K) [22,23]	$T_{\text{Boyle}}$ (K) [24]	$T_{\text{Boyle}}$ (K) [25]
R143a	805.40	762.13	
R152a	893.69	843.91	
R21	1079.19		
R218	782.00		
R22	876.42	836.04	
R227ea	837.62	781.54	
R23	696.17	658.80	
R236ea	908.33	845.09	
R236fa	877.59		
R245ca	997.38		
R245fa	943.84		
R32	812.25	766.61	
R41	761.81	730.02	
RC318	864.80		
Others			
Sulfur hexafluoride	760.41		
Toluene	1373.97		1452.28
Water	1448.82		1546.25
Acetone	1158.42		1222.11
Ammonia	945.81		1057.68
Benzene	1341.44		1435.62
Decafluorobutane	852.92		
Dodecafluorobutane	908.29		
Carbonyl sulfide	956.02		1516.65
Dimethylether	958.91		
Fluorine	374.63		
Hydrogen sulfide	940.64		906.63
Nitrogen trifluoride	582.17		

virial equation or the Zeno line. Holleran [21] has obtained Boyle temperatures of substances where the virial coefficient crosses zero using different parts of the Zeno line. He has found that the Boyle temperatures are different but they are within the maximum difference established in this work. This is an indication of the advantage of the linearity of the Zeno line since the extrapolation is obviously natural.

To test the accuracy of our calculations we have also compared our results with those obtained from second virial coefficients using the Tsonopoulos correlation [22,23], a modification of the Tsonopoulos correlation [24], and a correlation based upon square-well potential [25]. Table 2 shows the Boyle temperatures from these correlations. It is important to notice that the differences in the Boyle temperature from second virial correlations with similar functionality are higher than those obtained from EOS. For example, the maximum difference between the calculated Boyle temperature from the Tsonopoulos correlation [22,23], and the modified Tsonopoulos [24] is up to 100, 50, 60 K for hydrocarbons, gases and freons, respectively. In general, the modified Tsonopoulos correlation predicts lower temperatures than the original Tsonopoulos correlation. In the case of the correlation based upon the square-well potential, their Boyle temperatures agree with those from the Tsonopoulos correlations within 30 K for *n*-alkanes with  $n \leq 4$  and 113 K for *n*-alkanes with  $n > 4$ . For gases and other substances, the agreement in the Boyle temperature between both correlations is within 48 and 112 K, respectively.

Table 3

Maximum absolute difference in the calculation of the Boyle temperature from the Zeno line and different second virial correlations

Substances	Max $ \Delta T_{\text{Boyle}}^{(1)} $ (K)	Max $ \Delta T_{\text{Boyle}}^{(2)} $ (K)	Max $ \Delta T_{\text{Boyle}}^{(3)} $ (K)
Hydrocarbons	73	181	112
Gases	37	91	11
Alcohols	401		382
Freons	63	99	
Others	151		109

$\Delta T_{\text{Boyle}}^{(1)} = T_{\text{Boyle}}(\text{Zeno Line}) - T_{\text{Boyle}}(\text{Tsono})$ , Tsonopoulos [22,23];  $\Delta T_{\text{Boyle}}^{(2)} = T_{\text{Boyle}}(\text{Zeno Line}) - T_{\text{Boyle}}(\text{Mod. Tsono})$ , Meng et al. [24];  $\Delta T_{\text{Boyle}}^{(3)} = T_{\text{Boyle}}(\text{Zeno Line}) - T_{\text{Boyle}}(\text{SW})$ , McFall et al. [25].

The maximum difference between the Boyle temperatures obtained from the Zeno line and from the second virial correlations are shown in Table 3. The Boyle temperatures obtained from this work have a better agreement with the original Tsonopoulos correlation than with the other two correlations, as shown in Table 3. The only substances where we found high discrepancies between Boyle temperatures using different procedures are ethanol, 1-propanol and water.

A concern could also exist about a better calculation of the Boyle temperature using calculated virial coefficients from an interaction pair potential. Vega and López-Rodríguez [20] has used molecular simulations to calculate the Boyle temperature of *n*-alkanes from second virial coefficients calculations using an interaction pair potential based upon the rotational isomeric state approximation. Their calculation of the second virial coefficient depends upon four parameters for the pair potential. They obtained differences in the calculation of the Boyle temperature of an average value of 50 K when they considered constant all the parameters of the pair potential except one, the reduced energy parameter for the interaction of  $\text{CH}_2\text{-CH}_2$ . They changed this parameter only by two units. For example, we have calculated for octane a value between 1300 and 1311 K and they have calculated a value of 1298 and 1257 K. The Tsonopolous correlation gives a value of 1246 K. They stated that the experimental value is 1309 K. Recently, McLure and co-workers [26,27] used the approximate nonconformal (ANC) theory to obtain parameters for an interaction pair potential. They used it to calculate second virial coefficients and Boyle temperatures. Their values for non-polar substances agree with our calculations within an average value of 20 K.

## 5. Conclusions

We have determined the Boyle temperature of 83 pure substances using accurate EOS. The values of these temperatures vary within 63 K depending upon the EOS and the group of substances. We have shown that the Boyle temperatures calculated from correlations for the second virial coefficient are not better than those calculated from the Zeno line and higher differences can occur among them when calculating the Boyle temperature. Also, we have shown that EOS, although highly accurate, can predict a spurious Zeno line inside the equilibrium dome.



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