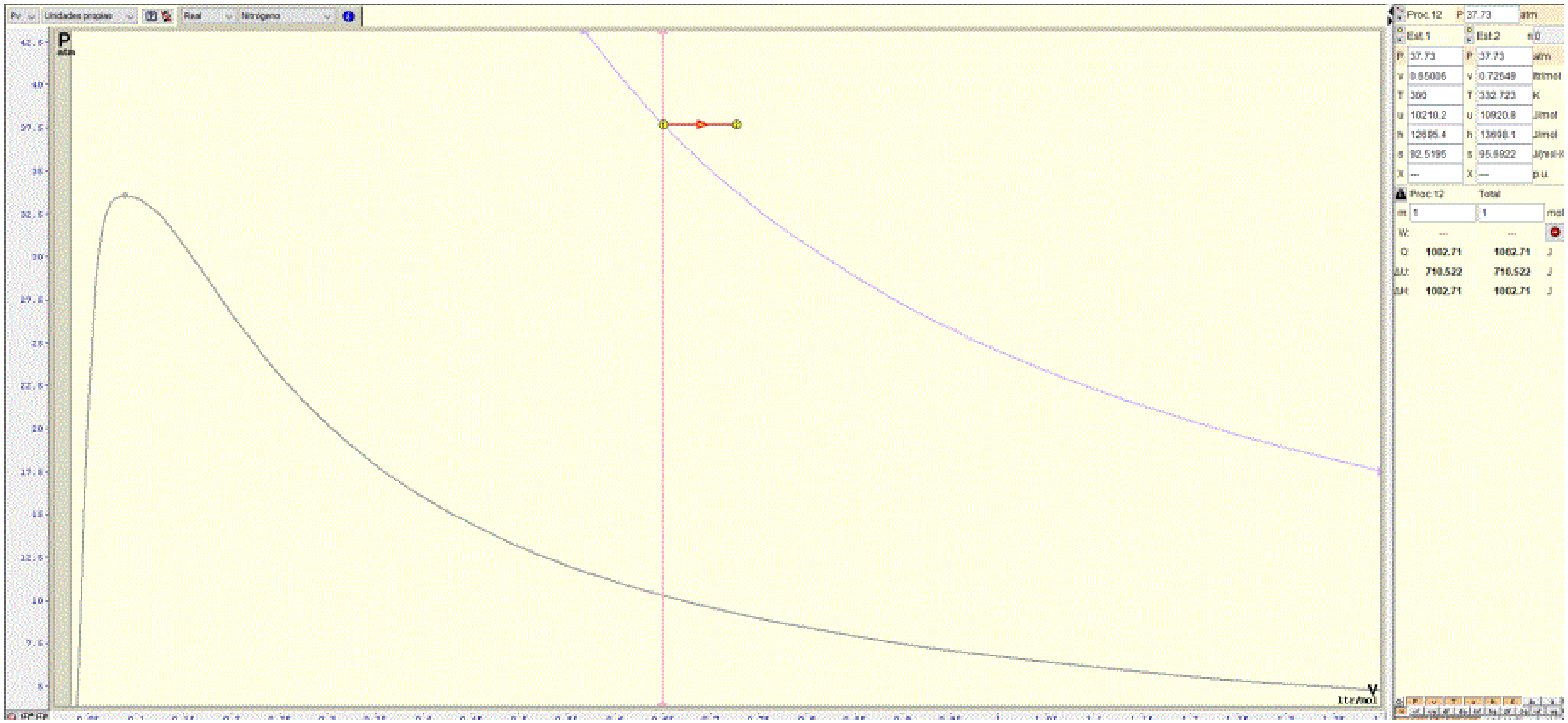
Clase 70 4 Enero 2021

Título de la nota 15/12/2020



1	**Obtención de la presión de un gas con el modelo tipo Clausius**	
2	Introducir los valores en las celdas de color amarillo	
3	Tc (K)	126.15
4	V sistema(L/mol)	0.6500
5	pc (atm)	33.5400
6	a (atmL^{2}K/mol^2)	169.7893
7	b (L/mol)	0.0130
8	R (atmL/molK)	0.082
9	T sistema(K)	300.00
10	c (L/mol)	0.0256
11	Vc (L/mol)	0.0901
12		
13	p ideal (atm)	37.8462
14	p real (atm)	37.3781
15		
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Modelo

$$P = \frac{RT}{(\bar{V}-b)} - \left[\frac{a}{(\bar{V}+c)^2 T}\right]$$

	A	B	C
1	**Obtención de la presión de un gas con el modelo tipo Redlich-Kwong**		
2	Introducir los valores en las celdas de color amarillo		
3	Tc (K)		126.26
4	V sistema (L/mol)		0.6500
5	pc (atm)		33.5400
6	a (atmL^{2}K$^{0.5}$/mol^2)		15.3628
7	b (L/mol)		0.0268
8	R (atmL/molK)		0.082
9	T sistema(K)		300.00
10			
11			
12			
13	p ideal (atm	37.8462	
14	p real (atm)	37.4550	
15			
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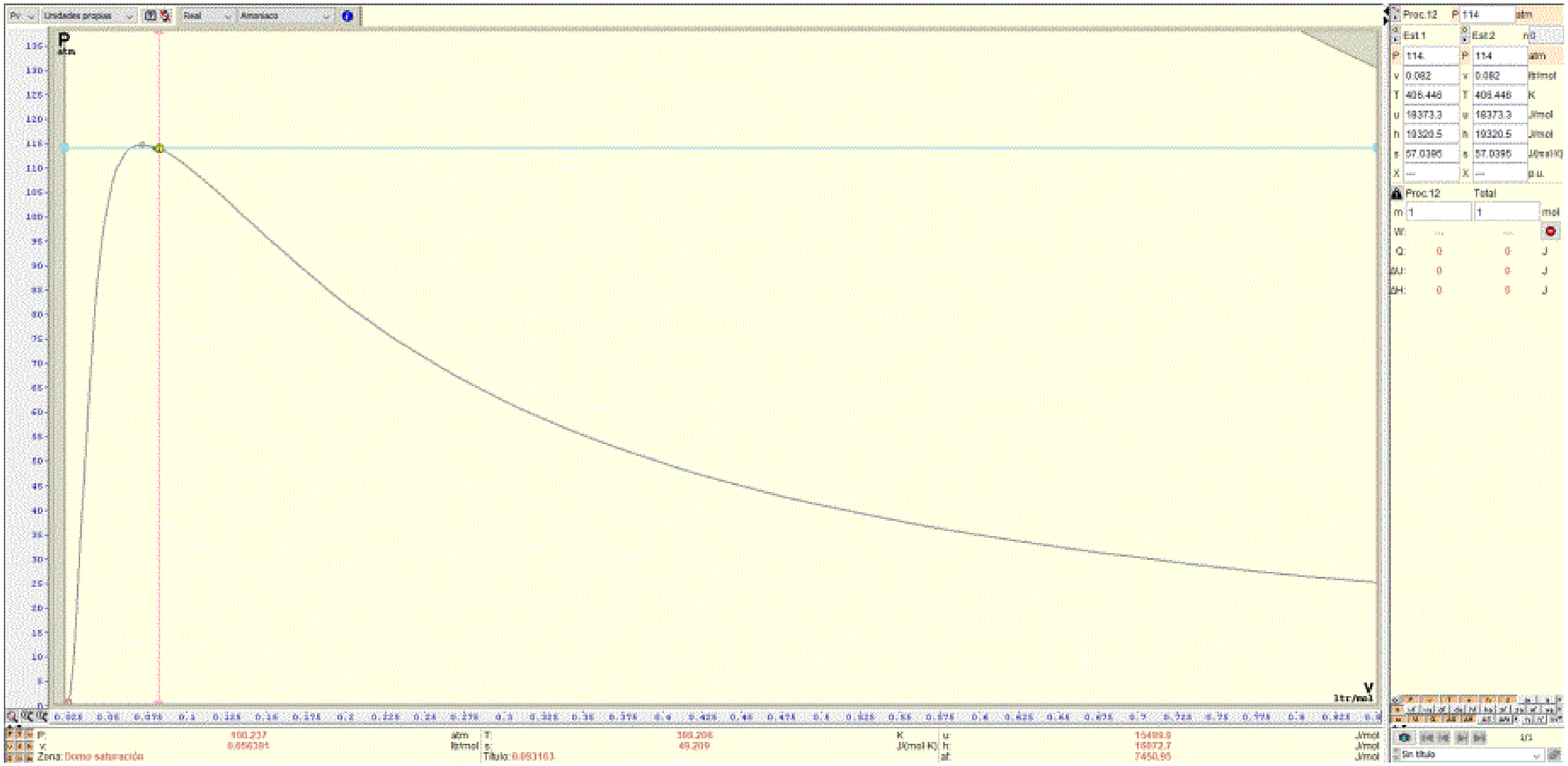
17			

Modelo

$$P = \frac{RT}{(\bar{V}-b)} - \left[\frac{a}{(\bar{V}^2+\bar{V}b)T^{0.5}}\right]$$



Obtención de ecuación cúbica de la temperatura tipo Redlich-Kwong

Introducir los valores en las celdas de color amarillo

Tc (K)	405.6000
V (L/mol)	0.0820
pc (atm)	111.3000
p sistema (atm)	114.0000
a (atmL²K^0.5/mol²)	85.6285
b (L/mol)	0.0259
R (atmL/molK)	0.082

Modelo 2

$$T^3 - T\frac{\left[p^2\left(\bar{V}-b\right)^2\right]}{R^2} - \frac{a^2\left(\bar{V}-b\right)^2}{R^2\left(\bar{V}^2+\bar{V}b\right)^2} = 0$$

T^3	T^2	T	Cte
1	0	-6081.1000	-43820057.1337

T ideal (K)	114.0000
T real (K)	358.302

Resolución de la ecuación tipo $AT^3+BT^2+CT+D=0$

Obtención de ecuación cúbica de la temperatura tipo Clausius

Introducir los valores en las celdas de color amarillo

Tc (K)	405.60
V sistema (L/mol)	0.08
pc (atm)	111.3000
p sistema (atm)	114.0000
a (atmL²K/mol²)	1700.6313
b (L/mol)	-0.0022
R (atmL/molK)	0.082
c (L/mol)	0.0396
Vc (L/mol)	0.0725

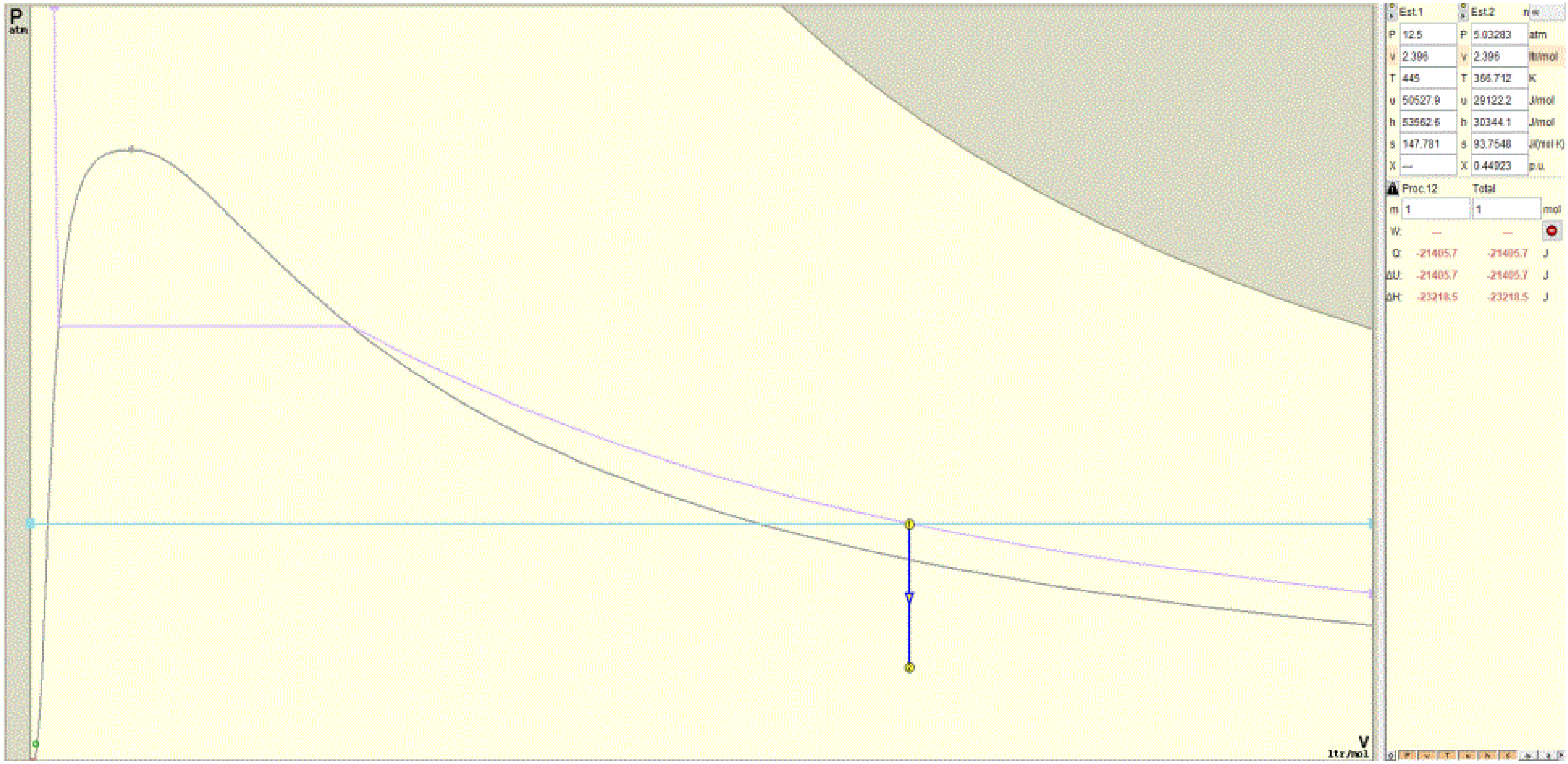
Modelo

$$T^2 - T\left(\frac{\bar{V}p - pb}{R}\right) - \frac{a\left(\bar{V}-b\right)}{R\left(\bar{V}+c\right)^2}$$

T^2	T	Cte
1.0000	-117.0672	-118185.4487

T ideal (K)	114.0000
T real (K)	407.2622

Resolución de la ecuación tipo $AT^2+BT+C=0$



Obtención de la ecuación cúbica del volumen modelo Clausius

Introducir los valores en las celdas de color amarillo

Tc (K)	469.60
T sistema (K)	445.00
pc (atm)	33.3000
p sistema (atm)	12.5000
a (atmL^{2}K/mol^2)	8821.6846
b (L/mol)	0.0149
R (atmL/molK)	0.082
c (L/mol)	0.1296
Vc (L/mol)	0.3040

Modelo

$$\bar{V}^3+\bar{V}^2\left[2c-b-\frac{RT}{p}\right]+\bar{V}\left[c^2-\frac{2cRT}{p}-2cb+\frac{a}{pT}\right]-\left[c^2\left(b+\frac{RT}{p}\right)+\frac{ab}{pT}\right]=0$$

V^3	V^2	V	Cte
1.0000	-2.6748	0.8420	-0.0730

V ideal (L/mol)	2.9192
V real (L/mol)	2.3264

Obtención de la ecuación cúbic[redacted]umen modelo Redlich-Kwong

Introducir los valores en las celdas de color amarillo

Tc (K)	469.60
T sistema (K)	445.00
pc (atm)	33.3000
p sistema (atm)	12.5000
a (atmL^{2}K$^{0.5}$/mol^2)	412.8045
b (L/mol)	0.1003
R (atmL/molK)	0.082

Modelo

$$\bar{V}^3-\bar{V}^2\left[\frac{RT}{p}\right]-\bar{V}\left[b^2+\frac{bRT}{p}-\frac{a}{pT^{0.5}}\right]-\left[\frac{ab}{pT^{0.5}}\right]=0$$

V^3	V^2	V	Cte
1.0	-2.9192	1.2628	-0.1570

V ideal (L/mol)	2.9192
V real (L/mol)	2.4252

Z { avance de Van der Waals

generalizada { variables reducidas

$$= \frac{\bar{V}\ \text{real}}{\bar{V}\ \text{ideal}} = 1$$

> 1 repulsión

< 1 atracción

$$\boxed{pV = ZnRT}$$

$$\boxed{p\bar{V} = ZRT}$$

Variables reducidas (adimensionales)

$$T_r = \frac{T_{sis}}{T_c} \qquad p_r = \frac{p_{sis}}{p_c}$$

$$V_r = \frac{\bar{V}_{sis}}{\bar{V}_c}$$

densidad $\rho = \frac{m}{V}$

$$Z = \frac{P\bar{V}}{RT} \qquad P = \frac{RT}{\bar{V}-b} - \frac{a}{\bar{V}^2}$$

$$Z = \frac{\bar{V}P}{RT} = \frac{\bar{V}}{RT}\left[\frac{RT}{\bar{V}-b} - \frac{a}{\bar{V}^2}\right]$$

$$Z = \frac{\bar{V}}{\bar{V}-b} - \frac{a}{\bar{V}RT} \qquad \frac{\bar{V}}{\bar{V}-b} = \frac{1}{1-\frac{b}{\bar{V}}}$$

$$\frac{1}{1-\frac{b}{\bar{V}}} = 1 + \frac{b}{\bar{V}} + \left(\frac{b}{\bar{V}}\right)^2 + \left(\frac{b}{\bar{V}}\right)^3 \cdots\cdots$$

$$Z = 1 + \frac{b}{\bar{V}} + \left(\frac{b}{\bar{V}}\right)^2 + - \frac{a}{\bar{V}RT}$$

$$\boxed{= 1 + \frac{1}{\bar{V}}\left[b - \frac{a}{RT}\right]} + \frac{b^2}{\bar{V}^2} + \ldots$$

$$\frac{1}{\bar{V}} = \frac{P}{RTz} \qquad P\bar{V} = ZRT$$

$$Z = 1 + \frac{1}{RTz}\left[b - \frac{a}{RT}\right]P + \left[\frac{b^2}{R^2T^2z^2}\right]P^2$$

$$\boxed{Z = 1 + \boxed{\frac{1}{RT}\left[b - \frac{a}{RT}\right]P}}$$

a p bajo $Z = 1$ $\quad Z = f(T, P)$

$$\left(\frac{\partial Z}{\partial P}\right)_T = \boxed{\frac{1}{RT}\left[b - \frac{a}{RT}\right]}$$

$\downarrow$ Segundo coeficiente virial.

$$\boxed{b - \frac{a}{RT_B} = 0}$$

T_B: Temp. de Boyle

$$Z = \frac{P\bar{V}}{RT} = 1 + \frac{1}{\bar{V}}\left[b - \frac{a}{RT}\right]$$

$$P\bar{V} = RT\left\{1 + \frac{1}{\bar{V}}\left[b - \frac{a}{RT}\right]\right\}$$

$$b = \frac{R}{8}\frac{T_c}{P_c}$$

$$a = \frac{27}{64}\frac{R^2 T_c^2}{P_c}$$

$$b - \frac{a}{RT_B} = 0$$

$$T_B = \frac{a}{bR} = \frac{\frac{27/64\, R^2 T_c^2}{P_c}}{\frac{RT_c}{8P_c} R}$$

$$\boxed{T_B = \frac{27}{8} T_c}$$

$$P\bar{V} = RT\left[1 + \frac{B(T)}{\bar{V}} + \frac{C(T)}{\bar{V}^2} + \frac{D(T)}{\bar{V}^3}\right]$$

Kammerligh - Onnes (ec. virial)

$$\boxed{Z = 1 + \boxed{\frac{B(T)}{\bar{V}}} + \boxed{\frac{C(T)}{\bar{V}^2}} + \boxed{\frac{D(T)}{\bar{V}^3}}}$$

$$\boxed{Z = 1 + B'(T)p + C'(T)p^2 + D'(T)p^3}$$

$$\boxed{Z = 1 + \frac{B(T)}{\bar{V}} + \frac{C(T)}{\bar{V}^2} + \frac{D(T)}{\bar{V}^3}}$$

$$B' = \frac{B}{RT} \quad C' = \frac{C - B^2}{R^2T^2} \quad D' = \frac{D - 3BC - 2B^3}{R^3T^3}$$

$$B' = \frac{(L/\cancel{mol})}{\frac{atm\,L}{\cancel{mol}\,\cancel{K}}\cancel{K}} = atm^{-1}$$

$$C' = atm^{-2} \quad D' = atm^{-3}$$

$$Z = 1 + \boxed{B'(T)}\,p + \boxed{C'(T)}\,p^2 + \boxed{D'(T)}\,p^3$$

$$= 1 + \frac{1}{atm}(atm) + \frac{1}{atm^2}\,atm^2 + \frac{1}{atm^3}\,atm^3$$

$$= \text{adimensional}$$

$$Z = 1 + \frac{B(T)}{\bar{V}} + \frac{C(T)}{\bar{V}^2} + \frac{D(T)}{\bar{V}^3}$$

$$1 + \frac{L/mol}{L/mol} + \frac{(L/mol)^2}{(L/mol)^2} + \frac{(L/mol)^3}{(L/mol)^3}$$

Calcular a y b de un gas real a 0°C si la $T_B = 107\ K$ • $Z_1 = 1.00054$ $P = 1\ atm$.

$$Z = 1 + \frac{1}{RT}\left[b - \frac{a}{RT}\right]P$$

$$T_B = \frac{a}{bR} \qquad a = T_B b R$$

$$Z = 1 + \frac{1}{RT}\left[b - \frac{T_B b \cancel{R}}{\cancel{R} T}\right]P$$

$$1.00054 = 1 + \frac{1}{RT}\left[b - \frac{T_B b}{T}\right]P$$

$$1.00054 = 1 + \frac{1}{\left(\frac{0.082\,\cancel{atm}\,L}{mol\,\cancel{K}}\right)\left(273.15\,\cancel{K}\right)}\left[b - \frac{107\,\cancel{K}\,b}{273.15\,\cancel{K}}\right]1\,\cancel{atm}$$

$$\boxed{b = \frac{L}{mol} = 0.01988\ \frac{L}{mol}}$$

$$\boxed{a = T_B b R = \left(107\,\cancel{K}\right)\left(\frac{0.01988\,L}{mol}\right)\left(0.082\,\frac{atm\,L}{mol\,\cancel{K}}\right) = 0.1744\ \frac{atm\,L^2}{mol^2}}$$

Propiedades Fisicoquímicas de sustancias

Nombre	neón	
Masa Molar	20.183	g/mol
Temperatura Crítica	44.400	K
Presion Crítica	27.200	atm
Volumen Crítico	0.0417	L/mol
Punto ebullición	27.000	K
Punto de fusión	24.500	K
Cp (cal/mol K)	0.000e+0	a
$Cp=a+bT+cT^2+dT^3$	0.000e+0	b
(300-2500)K	0.000e+0	c
	0.000e+0	d
Constantes de Antonio	14.0099	A
LN(p)=A-(B/(T+C))	180.4700	B
T=K	-2.6100	C
p=mmHg		

FES ZARAGOZA

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Con apoyo del programa UNAM-DGAPA-PAPIME
PE-200419

iedades | Obtención de a y b

Obtención de a y b de Van der Waals

Modelo

$$p = \frac{RT}{\left(\overline{V}-b\right)} - \left[\frac{a}{\overline{V}^2}\right]$$

R (atmL/molK)

0.082

Modelo

$$a = 3pc\overline{Vc}^2 \qquad b = \frac{\overline{Vc}}{3}$$

a	$atmL^2/mol^2$	0.14189
b	L/mol	0.01390

Independiente de volumen crítico

Modelo

$$a = \frac{27R^2Tc^2}{64pc} \qquad b = \frac{RTc}{8pc}$$

a	$atmL^2/mol^2$	0.20559
b	L/mol	0.01673

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$$\boxed{\begin{array}{l} Z = 1 + \dfrac{1}{RT}\left[b - \dfrac{a}{RT}\right]P \\ \\ T = 107 \quad Z = 1 \\ \\ T = 273.15 \quad Z = 1.00054 \end{array}}$$

T 53K

$Z < 1$