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دانشکده مهندسی شیمی - پردیس دانشکده‌های فنی - دانشگاه تهران  
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Huron-Vidal

(PR) (SRK)

(Huron-Vidal ) C<sub>2</sub>

Chrastil Mendez

Charstil, Aguilera, Gordillo, Mendez

SRK, PR

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(% AARD)

$$AARD(\%) = \frac{1}{n} \sum \left| \frac{y_{2,\text{exp}} - y_{2,\text{calv}}}{y_{2,\text{exp}}} \right| \times 100 \quad ( )$$

n

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Solute	M [g/mol]	P <sub>c</sub> [MPa]	T <sub>c</sub> [K]	$\omega$	A	B [K]	V <sup>sol</sup> *10 <sup>3</sup> [m <sup>3</sup> /mol]
Phenanthrene	178.24	3.17	882.55	0.3299	14.631	4873.4	0.1512
Benzoic Acid	122.124	4.50	752.00	0.620	14.408	4618.1	0.0965
Hexachloroethane	236.74	3.45	714.60	0.1630	10.6322	2600.94	0.1132
Triphenylmethane	244.34	2.24	863.00	0.5760	14.7858	5228.0	0.2409
Naphthalene	128.174	4.05	748.15	0.3020	13.583	3733.9	0.1103
2,3-dimethynaphtalene	156.23	3.22	785.00	0.4240	14.0646	4302.5	0.1547
2,6-dimethynaphtalene	156.23	3.22	777.00	0.4201	14.4286	4419.5	0.1547
Fluorene	166.23	2.99	821.00	0.4070	14.2046	4561.8	0.1393
Anthracene	178.234	3.12	869.30	0.3531	12.147	4397.6	0.1426
Pyrene	202.25	2.61	936	0.509			0.6299
Ascorbyl Palmitate	414.50	1.156	870.81	1.85	-	-	0.3405
BHA	180.2	2.883	798.78	0.63	-	-	0.1688
Dodecyl Gallate	338.45	1.846	905.90	1.20	-	-	0.2679
Propyl Gallate	170.12	4.772	862.87	0.86	-	-	0.155

Mendez	Chrastil
$T \ln(yP) = A' + B' \rho + C' T \quad (1)$ <p style="text-align: center;"><math>A', B', C'</math></p>	<p style="text-align: center;">Chrastil</p> <p style="text-align: center;"><math>AB_k</math></p>
$k = n_1 T + m_1 \quad (2)$ $B' = n_2 T + m_2 \quad (3)$	$\ln S_2 = k \ln \rho + \frac{\alpha}{T} + \beta \quad (4)$ <p style="text-align: center;"><math>\beta</math></p> <p style="text-align: center;"><math>\alpha</math></p>
<p style="text-align: center;">Chrastil</p> $\ln S_2 = (n_1 T + m_1) \ln \rho + \frac{\alpha}{T} + \beta \quad (5)$	<p style="text-align: center;">Del valle and Aguilera</p> <p style="text-align: center;">Chrastil</p> <p style="text-align: center;">Del valle and Aguilera</p>
<p style="text-align: center;">Mendez</p> $T \ln(y_2 P) = A' + (n_2 T + m_2) \rho + C' T \quad (6)$	$\ln S_2 = k \ln \rho + \frac{\alpha_1}{T} + \frac{\alpha_{11}}{T^2} + \beta \quad (7)$ <p style="text-align: center;"><math>k, \alpha_1, \alpha_{11}, \beta</math></p>
<p>EvIEWS 3.1</p>	<p style="text-align: center;">Del valle and Aguilera Chrastil</p>
	<p style="text-align: center;"><b>Gordillo</b></p> <p style="text-align: center;">Gordillo</p> $\ln(y_2) = D_0 + D_1 P + D_2 P^2 + D_3 P T + D_4 T + D_5 T^2 \quad (8)$ <p style="text-align: center;"><math>D_0, D_1, D_2, D_3, D_4, D_5</math></p> <p style="text-align: center;">Mendez-Santiago and Teja</p>

$$a_c = \eta_2 \frac{R^2 T_c^2}{P_c} \quad ( )$$

Chrastil

$$\alpha(T_r) = [1 + m(1 - \sqrt{T_r})]^2 \quad ( )$$

$$m_1 = \lambda_1 + \lambda_2 \omega + \lambda_3 \omega^2 \quad ( )$$

Chrastil

$n_1 T \ln \rho$

$\eta_1, \eta_2, \lambda_1, \lambda_2, \lambda_3$

Aguilera

(GCM)

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$$y_2 = \frac{f_2^{OS}}{\phi_2^v P} = \frac{P_2^{Sub}}{P} \frac{\exp\left(\frac{v_2^S (P - P_2^{Sub})}{RT}\right)}{\phi_2^v} \quad ( )$$

Huron and Vidal

$C_2$

PR SRK

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$$P = \frac{RT}{v-b} - \frac{a}{v(v+b)} \quad ( )$$

$$P = \frac{RT}{v-b} - \frac{a}{v(v+b) + b(v-b)} \quad ( )$$

Huron and Vidal

$$B_m = \sum y_i B_i = y_1 B_1 + y_2 B_2 \quad ( )$$

$b, a$

$$\frac{A_m}{B_m} = \sum y_i \left( \frac{A_i}{B_i} - \frac{\ln \gamma_i^\infty}{\ln 2} \right) = \sum_i y_i C_i \quad ( )$$

$$C_2 \quad ( )$$

$$C_2 = \frac{A_2}{B_2} - \frac{\ln \gamma_2^\infty}{\ln 2} \quad ( )$$

$$b = \eta_1 R \frac{T_c}{P_c} \quad ( )$$

$$a(T) = a_c \alpha(T_r) \quad ( )$$

$a_1, a_2, b_1, b_2$

$P_{ref}$

$C_2$

$C_2$

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Eviews 3.1 Matlab 7

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$C_2$

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Spiroindolinonaphthoxazine

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Coimbra

Chrastil

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$C_2$

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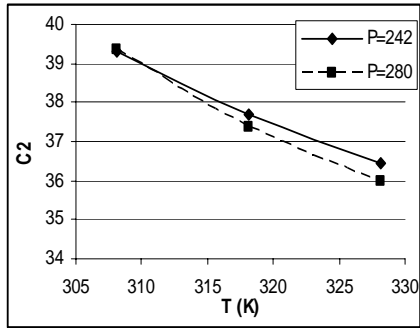
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$$C_2(T, P) = (a_1T + a_2) - (b_1T + b_2) \ln\left(\frac{P}{P_{ref}}\right) \quad ( )$$

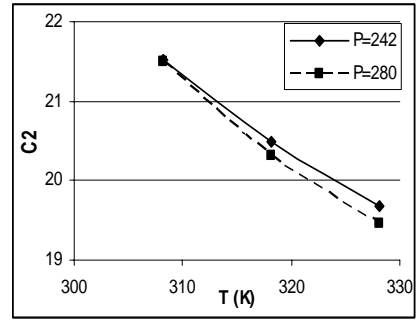
TBP

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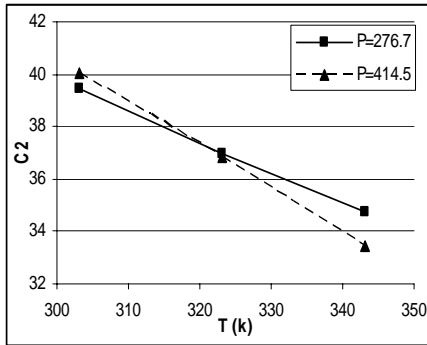
	Eq. (2)	Eq. (4)	Eq. (5)	Eq. (6)	Eq. (9)	Eq. (10)
Anthracene- CO <sub>2</sub>	18.04	14.02	37.59	29.30	17.83	28.04
Anthracene-Ethane	9.94	9.47	7.09	13.75	9.30	13.11
Fluorene- CO <sub>2</sub>	21.72	17.30	73.85	32.93	21.70	32.52
Fluorene-Ethylene	8.10	6.67	49.97	35.75	6.91	21.87
Naphthalene-Ethane	13.93	14.27	83.96	16.19	11.40	15.43
Triphenylmethane- CO <sub>2</sub>	9.65	7.32	21.49	10.87	8.90	10.94
Pyrene- CO <sub>2</sub>	23.43	23.38	59.24	44.54	20.28	34.78
Pyrene-ethylene	7.98	-	-	34.99	7.93	22.12
Phenantrene-CO <sub>2</sub>	5.86	5.74	10.12	9.44	4.28	5.15
Phenanthrene-C <sub>2</sub> H <sub>4</sub>	11.15	9.04	8.92	10.22	10.63	7.34
Phenantrene-Ethylene	2.55	1.34	0.00	1.58	1.39	1.27
Dodecyl Gallate- CO <sub>2</sub>	5.58	-	-	6.28	1.50	2.61
Propyl Gallate- CO <sub>2</sub>	3.60	-	-	4.85	2.29	2.28
Ascorbyl Palmitate- CO <sub>2</sub>	5.07	-	-	3.77	-	3.38
Butyl Hydroxyl Anisole- CO <sub>2</sub>	8.30	-	0.00	10.06	3.78	4.74
2,6-Dimethylnaphthalene-C <sub>2</sub> H <sub>4</sub>	10.03	9.37	18.35	12.80	10.39	6.40
2,6-Dimethylnaphthalene-CO <sub>2</sub>	9.38	9.36	23.16	15.54	8.89	9.01
2,3-Dimethylnaphthalene-CO <sub>2</sub>	13.19	13.00	21.32	18.00	11.65	15.08
Benzoic acid-CO <sub>2</sub>	9.81	9.67	11.74	16.16	9.22	9.54
Hexachloroethane-CO <sub>2</sub>	15.30	15.29	16.99	15.63	14.53	10.26
Benzoic acid-C <sub>2</sub> H <sub>4</sub>	8.88	9.01	7.93	12.42	8.86	11.69
<b>%Average</b>	<b>12.07</b>	<b>11.71</b>	<b>34.89</b>	<b>19.89</b>	<b>11.17</b>	<b>15.70</b>



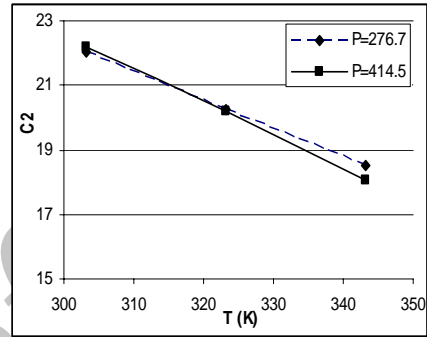
PR-EOS  
C<sub>2</sub> :



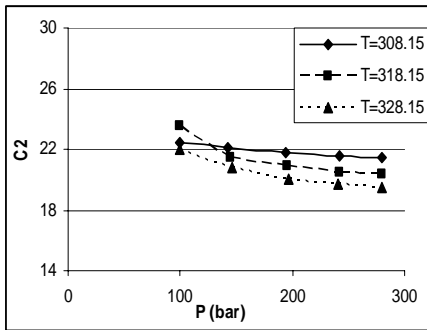
SRK-EOS  
C<sub>2</sub> :



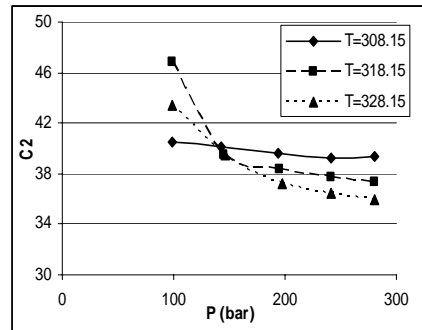
PR-EOS  
C<sub>2</sub> :



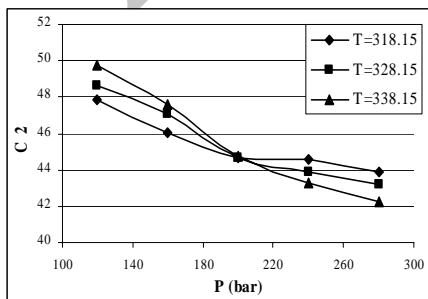
SRK-EOS  
C<sub>2</sub> :



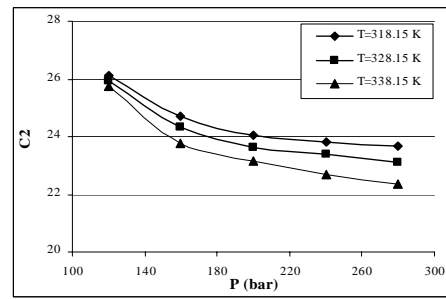
SRK-EOS  
C<sub>2</sub> :



PR-EOS  
C<sub>2</sub> :



PR-EOS  
C<sub>2</sub> :



SRK-EOS  
C<sub>2</sub> :

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**PR-EOS** ( ) :

	$a_1$	$a_2$	$b_1$	$b_2$	$P_{ref}$
Anthracene- CO <sub>2</sub>	-11.71061	0.15181	-48.41242	0.15445	90.6
Anthracene-Ethane	63.95572	-0.06400	13.74482	0.04552	104.3
Fluorene- CO <sub>2</sub>	31.57406	0.01874	-22.25118	0.07381	69.9
Fluorene-Ethylene	119.24868	-0.21770	11.15511	-0.02282	69.9
Naphthalene-Ethane	26.87023	0.03461	-38.78105	0.13394	35.4
Pyrene- CO <sub>2</sub>	53.40834	0.00055	-14.19848	0.05861	104.3
Pyrene-ethylene	126.54046	-0.19651	12.68261	-0.02073	104.8
Phenanthrene- CO <sub>2</sub>	0.22600	-67.38105	0.11201	11.77612	80.9
Phenanthrene-C <sub>2</sub> H <sub>4</sub>	77.64750	-0.06460	-32.58310	0.12384	120
Phenanthrene-Ethlene	106.85941	-0.24870	50.96796	-0.17492	276.8
Triphenylmethane-Ethane	56.221648	-0.00221	-72.679333	0.24111	69.9
Ascorbyl Palmitate- CO <sub>2</sub>	44.22489	-0.10575	271.25330	-0.91581	130
BHA- CO <sub>2</sub>	-46.75261	0.28427	-198.29651	0.62973	150
Dodecyl Gallate- CO <sub>2</sub>	-363.61649	1.33476	-293.29176	0.95057	150
Propyl Gallate- CO <sub>2</sub>	-221.55230	0.82812	-224.46840	0.71513	150
2,3-Dimethylnaphthalene- CO <sub>2</sub>	5.58520	0.11695	-22.60553	0.07780	99
2,6-Dimethylnaphthalene- C <sub>2</sub> H <sub>4</sub>	120.13071	-0.22341	17.76860	-0.03965	80
2,6-Dimethylnaphthalene- CO <sub>2</sub>	-12.20245	0.17150	-89.03309	0.297778	97
Benzoic acid- C <sub>2</sub> H <sub>4</sub>	98.70964	-0.14387	-4.21413	0.00493	120
Benzoic acid- CO <sub>2</sub>	47.35324	0.01744	-35.37715	0.13352	120
Hexachloroethane- CO <sub>2</sub>	-5.43943	0.10441	-46.73699	0.15133	99

**SRK-EOS** ( ) :

	$a_1$	$a_2$	$b_1$	$b_2$	$P_{ref}$
Anthracene- CO <sub>2</sub>	22.36295	-0.00874	-10.98372	0.03450	90.6
Anthracene-Ethane	40.01947	-0.05203	-3.94254	0.01390	104.3
Fluorene- CO <sub>2</sub>	35.06430	-0.04513	-5.16126	0.01858	69.9
Fluorene-Ethylene	64.41210	-0.11899	6.78220	-0.01549	69.9
Naphthalene-Ethane	13.89840	0.02383	-19.27564	0.06826	35.4
Pyrene- CO <sub>2</sub>	53.03783	0.00055	-14.19848	0.05861	104.3
Pyrene-ethylene	64.38652	-0.09852	2.62839	0.00007	104.8
Phenanthrene- C <sub>2</sub> H <sub>4</sub>	48.06919	-0.05757	-6.56959	0.02949	120
Phenanthrene-CO <sub>2</sub>	0.05001	-13.31905	-0.02305	33.15711	80.9
Phenanthrene-Ethlene	58.23523	-0.13545	28.75895	-0.09792	276.8
Triphenylmethane-Ethane	48.62361	-0.05926	-20.99134	0.07141	69.9
Ascorbyl Palmitate- CO <sub>2</sub>	25.88340	-0.06179	138.06860	-0.46581	130
BHA- CO <sub>2</sub>	-18.73836	0.13650	-72.01950	0.22990	150
Dodecyl Gallate- CO <sub>2</sub>	-129.90112	0.51080	-80.72521	0.26513	150
Propyl Gallate- CO <sub>2</sub>	-79.57368	0.31978	-73.42003	0.233622	150
2,3-Dimethylnaphthalene- CO <sub>2</sub>	30.73873	-0.02595	-22.60553	0.077795	99
2,6-Dimethylnaphthalene- C <sub>2</sub> H <sub>4</sub>	60.94417	-0.11113	8.87989	-0.021756	80
2,6-Dimethylnaphthalene- CO <sub>2</sub>	18.41990	0.01194	-25.81840	0.08807	97
Benzoic acid- C <sub>2</sub> H <sub>4</sub>	55.57447	-0.08914	6.67402	-0.01351	120
Benzoic acid- CO <sub>2</sub>	52.18188	-0.07855	9.16441	-0.02103	120
Hexachloroethane- CO <sub>2</sub>	11.77513	0.01132	-7.38065	0.02559	99

Chrastil

(% / )

Gordillo

(% / )

Chrastil

$n_1 T \ln \rho$

Aguilera

(C<sub>2</sub> )

C<sub>2</sub>

C<sub>2</sub>

C<sub>2</sub>

$T$	
$T_c$	$f_2^{OS}$
$T_r$	$M_w$
$V_2^S$	$N$
$y_2$	$P$
$\phi_i$	$P_c$
$\rho$	$P_r$
$\gamma_i^\infty$	$P_2^{Sub}$
	$R$
	$S_2$

( )

	SRK-EOS	PR-EOS	N
Anthracene- CO <sub>2</sub>	17.22	15.73	23
Anthracene-Ethane	7.78	8.18	27
Fluorene- CO <sub>2</sub>	10.02	11.59	30
Fluorene-Ethylene	21.07	30.16	24
Naphthalene-Ethane	30.34	42.44	23
Pyrene- CO <sub>2</sub>	16.41	26.07	21
Pyrene-ethylene	12.93	15.92	15
Phenanthrene- C <sub>2</sub> H <sub>4</sub>	15.74	20.25	15
Phenanthrene- CO <sub>2</sub>	9.87	9.30	21
Phenanthrene-Ethlene	3.02	2.94	6
Triphenylmethane- CO <sub>2</sub>	34.38	43.33	19
Ascorbyl Palmitate- CO <sub>2</sub>	6.32	6.41	8
BHA- CO <sub>2</sub>	16.50	29.52	6
Dodecyl Gallate- CO <sub>2</sub>	7.12	10.59	8
Propyl Gallate- CO <sub>2</sub>	3.98	6.00	8
2,3-Dimethylnaphthalene- CO <sub>2</sub>	8.86	22.62	15
2,6-Dimethylnaphthalene- C <sub>2</sub> H <sub>4</sub>	18.01	26.66	18
2,6-Dimethylnaphthalene- CO <sub>2</sub>	10.79	22.13	15
Benzoic acid- C <sub>2</sub> H <sub>4</sub>	3.35	4.29	15
Benzoic acid- CO <sub>2</sub>	5.93	13.53	15
Hexachloroethane- CO <sub>2</sub>	6.58	23.41	15
<b>%AARE</b>	<b>14.00</b>	<b>19.85</b>	-

%AARD

	Mendez	Chrastil	SRK-EOS	PR-EOS
Coimbra	6.3	7.9	28.14	24.65
	6.2	6.9	13.70	18.15

	Equation of state		Chrastil model	
	PR-EOS	SRK-EOS	Modified form	Main form
%AARD	17.01	8.97	5.99	6.40

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- 1- Super Critical Fluid Extraction  
2- Absolute Average Relative Deviation  
3- Group Contribution Method

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