

SYSTEM –

1Butanol & 1,2 Propanediol

Activity Coefficient Model –

Wilson

Type of Equation	Parameters	$\ln \gamma_1 =$ $\ln \gamma_2 =$	Notation of Parameters in Data Sheet
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Wilson [8]	$\lambda_{12} - \lambda_{11}^{(1)}$	$-\ln(x_1 + \Lambda_{12}x_2) + x_2 \left(\frac{\Lambda_{12}}{x_1 + \Lambda_{12}x_2} - \frac{\Lambda_{21}}{\Lambda_{21}x_1 + x_2} \right)$ (30a)	A 12
	$\lambda_{21} - \lambda_{22}$	$-\ln(x_2 + \Lambda_{21}x_1) - x_1 \left(\frac{\Lambda_{12}}{x_1 + \Lambda_{12}x_2} - \frac{\Lambda_{21}}{\Lambda_{21}x_1 + x_2} \right)$ (30b)	A 21

1) $\Lambda_{12} = \frac{V_2^L}{V_1^L} \exp - \frac{\lambda_{12} - \lambda_{11}}{RT}$ $\Lambda_{21} = \frac{V_1^L}{V_2^L} \exp - \frac{\lambda_{21} - \lambda_{22}}{RT}$

V_i^L molar volume of pure liquid component i. For values of V_i^L see Appendix A.

λ_{ij} interaction energy between components i and j $\lambda_{ij} = \lambda_{ji}$

Parameters are given in cal/mol with the gas.

2. Antoine Vapor Pressure Equation

The Antoine vapor pressure equation is used in the following form:

$$\log[p_i^0] = A - \frac{B}{t + C} \quad (70)$$

with $[p_i^0]$ vapor pressure of pure component i in mm Hg
 t temperature in degrees Celsius ($^{\circ}\text{C}$)

The Antoine constants A, B, and C are given with respective temperature regions (in $^{\circ}\text{C}$).

Note- Here it is log (Base 10).

Value of Constants

(1) 1-BUTANOL		C4H10O	
(2) 1,2-PROPANEDIOL		C3H8O2	
+++++ ANTOINE CONSTANTS		REGION +++++	CONSISTENCY
(1)	7.83800 1558.190	196.881 -1- 118 C	METHOD 1 +
(2)	8.95446 2692.187	255.210 45- 188 C	METHOD 2 +
PRESSURE= 730.00 MM HG (.973 BAR)			

CONSTANTS:	A12	A21	α_{12}	γ_1^∞	γ_2^∞	OBJECTIVE FUNCTION
MARGULES	.4129	.6873		1.51	2.03	.0384 G
VAN LAAR	-290.6946	846.3203		1.51	1.95	.0404 G
WILSON	764.6865	-226.3497	.2993	1.50	1.99	.0395 G

Please take data corresponding to Wilson

There is no α_{12} for Wilson.

T-X-Y Data

EXPERIMENTAL DATA		
T DEG C	X1	Y1
180.30	.0185	.1970
175.65	.0335	.3185
168.90	.0595	.4590
163.80	.0925	.5845
161.50	.1035	.6150
154.10	.1500	.7150
151.15	.1720	.7525
147.35	.2090	.7940
145.25	.2350	.8180
140.10	.3015	.8590
136.80	.3520	.8825
134.05	.4220	.9080
130.35	.5090	.9290
128.35	.5705	.9430
126.00	.6390	.9540
123.10	.7330	.9670
121.30	.8045	.9770
118.60	.9055	.9860

Take the molar volume from NIST Database. If not available there, please contact the TA's (Sandra and Krishna).

All data taken from Dechema Chemistry Data Series.