COMPONENTS:

- (1) Propane: C₃H₈; [74-98-6]
 Butane; C₄H₁₀; [106-97-8]
 2-Methylpropane; C₄H₁₀; [75-28-5]
- (2) Alcohols

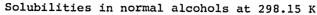
EVALUATOR:

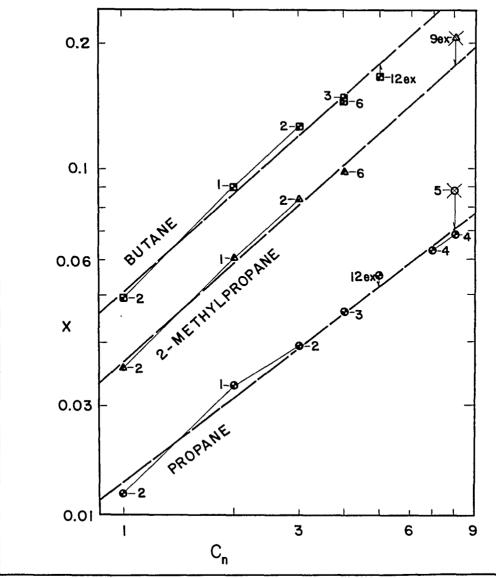
Walter Hayduk Department of Chemical Engineering University of Ottawa Ottawa, Canada KlN 9B4

January, 1984

CRITICAL EVALUATION:

Nine groups of workers have reported solubilities of propane, butane and 2-methylpropane in normal alcohols from methanol to octanol. In spite of the scarcity, there is a relatively high consistency for the data for all three gases. The sources of the data are listed separately for each gas; for propane: methanol (2), ethanol (1,10), butanol (3), heptanol (4) and octanol (4,5). The solubilities of propane in 2-propanol (2) and in 3-methyl-1-butanol (12) are compared with those in the normal alcohols. For butane: methanol (2,11), ethanol (1,13), butanol (3,6), and octanol (5). The solubilities of butane in 2-propanol (2) and 3-methyl-1-butanol (12) are also compared with those in the normal alcohols. Finally, for 2-methylpropane: methanol (2,11), ethanol (1), butanol (6), and octanol (9). These latter solubilities are compared with those in 2-propanol (2).





332

COMPONENTS:

- (1) Propane; C₃H₈; [74-98-6] Butane; C₄H₁₀; [106-97-8] 2-Methylpropane; C₄H₁₀ [75-28-5]
- (2) Alcohols

EVALUATOR:

Walter Hayduk Department of Chemical Engineering University of Ottawa Ottawa, Canada KlN 984

January, 1984

CRITICAL EVALUATION: continued

Solubilities for the three gases are shown for a temperature of 298.15 K and a gas partial pressure of 101.325 kPa in the diagram above in which the mole fraction solubility, x, and the number of carbon atoms in the solvent, \mathcal{C}_n , are shown on logarithmic scales. This method of obtaining a linear relation for solubilities in alcohols was previously used by Boyer and Bircher (14). It may be observed that the solubilities of all three gases in the tertiary alcohol 2-propanol (2), are completely consistent with the solubilities in the normal alcohols. Surprisingly, the early data of Friedel and Gorgeu (12) for propane and butane solubilities in 3-methyl-1-butanol correspond reasonably well to the expected solubilities in an alcohol of $\mathcal{C}_n = 5$, and are classified as tentative. On the other hand, the early data of Frankland (13) and Lebeau (10,11), although of historic interest, are all very much too low and are rejected. The solubilities of Gerrard (5,9) for propane and butane in octanol are both estimated to be at least 20% too high and are also rejected. The remaining data are classified as tentative (1,2,3,4,6). These latter data were used to determine regression lines (on logarithmic scales) for the three gases. Included were the solubilities in 2-propanol of Kretschmer and Wiebe (2).

For propane:

$$x_{C_3} = 0.01230 \ c_n^{0.7774}$$

Correlation coefficient = 0.997

For butane:

$$x_{C_4} = 0.04131 \ c_n^{0.9053}$$

Correlation coefficient = 0.996

For 2-methylpropane:

$$x_{iC_4} = 0.02625 \ c_n^{0.9128}$$

Correlation coefficient = 0.997

The above equations are represented as dashed lines in the diagram.

Three groups of workers have reported solubilities of propane, butane and 2-methylpropane in other alcohol solvents. The sources are listed separately for each gas; for propane: in 1,2-ethanediol (ethylene glycol)(7), 2-ethoxyethanol (ethylcellosolve)(8), oxybispropanol (dispropylene glycol)(7), phenol (7) and benzenemethanol (benzyl alcohol)(5,7), for butane: in 1,2-ethanediol (5), oxybispropanol (7), phenol (7), benzenemethanol (7) and 1,2,3-propanetriol (glycerol)(5), and for 2-methylpropane: in 1,2-ethanediol (7), 2-ethoxyethanol (8), phenol (7), benzenemethanol (9) and oxybispropanol (7). Unfortunately none of the above data is considered reliable enough to warrant classification as tentative; instead, they are all classified as doubtful for reasons that are discussed below. These data appear generally too high by an amount ranging from 5% to several factors and are considered of qualitative value only.

An explanation for the above classification follows. In the Critical Evaluation of the solubilities of *Ethane* in polar solvents (15) it was possible to directly compare some of the Lenoir et al. data (7) with those of four other workers. It was found that the Lenoir et al. data were from 6% to 46% higher than those of the other workers. The data in question here are from the same paper. In addition it was possible to compare hydrogen-bonding factors in 1-2-ethanediol for all

COMPONENTS:

- (1) Propane; C₃H₈; [74-98-6]
 Butane; C₄H₁₀; [106-97-8]
 2-methylpropane; C₄H₁₀;[75-28-5]
- (2) Alcohols

EVALUATOR:

Walter Hayduk Department of Chemical Engineering University of Ottawa Ottawa, Canada KlN 9B4

January, 1984

CRITICAL EVALUATION: continued

three gases (5,7) with those of several other gases which formed a consistent relation on a hydrogen-bonding factor diagram (16). For all three gases, the indicated solubilities yielded hydrogen-bonding factors much higher (> 20%) than expected. Although by no means conclusive by itself, this test is often effective in discerning inaccurate data. Hence, although copious, the data of Lenoir et al. (7) are classified as doubtful. In the first part of this Critical Evaluation, the data of Gerrard for the solubility of propane and butane in octanol (5) were considered to be too high by at least 20%. It is expected that while this order of error may be present for the solubility of propane in benzenemethanol, that it is probably much higher in the reported solubility of *butane* in 1,2-ethanediol. Mo hydrocarbon gases have a very low solubility in the highly polar 1,2-ethanediol so that the relatively high solubility indicated by Gerrard (5) appears several factors too high. Again sufficient doubt is associated with these data to warrant classification as doubtful. Finally, some doubt is also cast on the solubilities of Ezheleva and Zorin (8, in Russian) on examination of an example given in their paper explaining the method of data treatment. The example shows a linear plot of mole fraction solubility versus different values of gas partial pressure. When the resulting lines are extrapolated to zero partial pressure, they do not pass through the origin even approximately, but were nonetheless, apparently (incorrectly) used to evaluate Henry's law constants. If a similar method was followed in the calculation for other gas solubilities, large errors would have resulted. Hence, there appears to be reason to doubt the accuracy of the data for propane and 2-methylpropane in 2-ethoxyethanol (8).

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COMPONENTS:

- (1) Propane; C₃H₈; [74-98-6]
 Butane; C₄H₁₀; [106-97-8]
 2-methylpropane; C₄H₁₀; [75-28-5]
- (2) Alcohols

EVALUATOR:

Walter Hayduk Department of Chemical Engineering University of Ottawa Ottawa, Canada KlN 9B4

January, 1984

CRITICAL EVALUATION: continued

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- 15. Hayduk, W. Ed. IUPAC Solubility Data Series, Ethane, Pergamon Press, Oxford, England 1982, 9, 195-199.
- 16. Short, I.; Sahgal, A.; Hayduk, W. J. Chem. Eng. Data 1983, 28, 63-66.

335

COMPONENTS: (1) Propane; C₃H₈; [74-98-6] Kretschmer, C.B.; Wiebe, R. (2) Methanol; CH₄O; [67-56-1] J. Am. Chem. Soc. 1952, 74, 1276-7. VARIABLES: T/K = 273.15-323.15 P/kPa = 11.86-101.27 PREPARED BY: H.L. Clever W. Hayduk

EXPERIMENTAL VALUES:

T/K		essure /mm Hg Partial ²	Mole fraction 1,2	Ostwald Coefficient ² L/cm ³ cm ⁻³	Bunsen Coefficient ² α/cm ³ (STP)cm ⁻³ atm ⁻¹
	TOTAL	Faitlai	/x ₁	D/ CIII CIII	d/Ch (SIF/Ch ath
273.15	756.4	727.9 760.0	0.02039 0.0213	12.1	12.1
298.15	464.0 598.1 759.6	339.3 473.6 635.4	0.004988 0.007040 0.009569		
	, 55 (0	760.0	0.0115	6.88	6.37
323.15	758.4	346.2 760.0	0.003232 0.00709	4.46	3.73

¹Original data.

Mole fractions at 101.325 kPa were used to determine the following equation for $\ln x_1$ and table of smoothed values:

 $\ln x_1 = 1942.9/T - 10.9689$ Correlation coefficient = 0.9998

<i>T</i> /K	<u> </u>	<i>T</i> /K	x	
273.15	0.0212	303.15	0.0105	
283.15	0.0165	313.15	0.00853	
293.15	0.0130	323.15	0.00704	

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus was an all glass system which consisted of a monometer, gas handling system, gas buret and solubility bulb equipped with a magnetic stirrer.

The solubility bulb was evacuated and weighed. About 15 cm³ of solvent was distilled into the bulb, the solvent degassed and the bulb reweighed.

A sample of hydrocarbon was condensed into a calibrated tube; it was vaporized into a known volume and the pressure measured. Equilibrium was established between the gas and the solvent. Pressure was again measured.

A detailed description of the apparatus and values of the gas molal volume and 2nd virial coefficient are in (1).

SOURCE AND PURITY OF MATERIALS:

- (1) Phillips Petroleum Co., Research Grade. Specified 99.9 mole percent pure. Treated to remove dissolved gases and moisture.
- (2) Source not given. Treated to remove acetone and aldehydes. Fractionated through a 50-plate column, dried with Mg, stored in a sealed container. Density at 25°C 0.78653 g cm⁻³.

ESTIMATED ERROR:

 $\delta T/K = 0.005$

 $\delta p/\text{mm Hg} = 0.05$

 $\delta x_1/x_1 = 0.005$ (compilers)

REFERENCES:

Kretschmer, C.B.; Wiebe, R.
 J. Am. Chem. Soc. <u>1951</u>, 73, 3778.

²Calculations for 101.325 kPa (760 mm) were by compilers assuming Henry's law, and Raoult's law for solvent partial pressure.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propane; C ₃ H ₈ ; [74-98-6]	Kretschmer, C.B.; Wiebe, R.
(2) Ethanol; C ₂ H ₆ O; [64-17-5]	J. Am. Chem. Soc. 1951, 73, 3778-81
VARIABLES: T/K = 273.15-323.15 P/kPa = 33.10-101.91	PREPARED BY: H.L. Clever W. Hayduk

EXPERIMENTAL	WAY DEC.
P.XPP.RIMP.NIAL	VALUES:

<i>T/</i> K	_	ssure mm Hg Partial ²	Mole fraction 12 /x 1	Ostwald Coefficient ² L/cm ³ cm- ³	Bunsen Coefficient ² α/cm ³ (STP) cm ⁻³ atm ⁻¹
273.15	309.8 532.0 762.2	297.8 520.1 750.5	0.01497 0.02706 0.04054		
298.15	248.3 427.5 579.8 755.3	760.0 188.8 368.3 520.9 696.7	0.0411 0.005089 0.01003 0.01434 0.01941	16.5	16.5
323.15	412.0 596.4 764.4	760.0 191.1 376.2 544.9	0.0228 0.003201 0.006349 0.009245	9.55	8.71
	, , , ,	760.0	0.0129	5.67	4.75

continued

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus was an all-glass system which consisted of a manometer, gas handling system, gas buret and solubility bulb equipped with a magnetic stirrer.

The solubility bulb was evacuated and weighed. About 15 cm³ of solvent was distilled into the bulb, the solvent degassed and the bulb reweighed.

A sample of hydrocarbon was condensed into a calibrated tube; it was vaporized into a known volume and the pressure measured. Equilibrium was established between the gas and the solvent. Pressure was again measured.

SOURCE AND PURITY OF MATERIALS:

- (1) Phillips Petroleum Co. Research grade, 99.99 mole per cent. Removed dissolved air and moisture.
- (2) Commercial absolute alcohol sample fractionated, treated with Mg ethylate, stored in sealed container until used. Density, at 25°C 0.78505 g cm⁻³.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.005$

 $\delta p/\text{mmHg} = \pm 0.05$

 $\delta x_1/x_1 = \pm 0.005$ (compilers)

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Propane; C₃H₈; [74-98-6] Kretschmer, C.B.; Wiebe, R. (2) Ethanol; C₂H₆O; [64-17-5] J. Am. Chem. Soc. 1951, 73, 3778-81. VARIABLES: PREPARED BY: T/K = 273.15-323.15H.L. Clever P/kPa = 33.10-101.91W. Hayduk

EXPERIMENTAL VALUES: - concluded

Mole fractions at 101.325 kPa were used to determine the following equation for $\ln\,x_1$ and table of smoothed values:

 $\ln x_1 = 35.471 - 6.891 \ln T_1$ Correlation coefficient = 0.9998

<i>T/</i> K	<u>x</u>	<i>T</i> /K	<u>*1</u>	
273.15	0.0413	303.15	0.0201	
283.15	0.0322	313.15	0.0161	
293.15	0.0254	323.15	0.0130	
298.15	0.0226			

AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: ESTIMATED ERROR: REFERENCES:

¹Original data

 $^{^2\}mathrm{Calculations}$ for 101.325 kPa (760 mm) were by compilers by extrapolation of data from lower pressures, and by assuming Raoult's law for solvent partial pressure.

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Propane; C ₃ H ₈ ; [74-98-6]	Lebeau, P.	
(2) Water, Benzene, Ethanol, Diethylether, Chloroform, Turpentine	Compt. Rend. 1905, 140, 1454-6 and 1572. Bull. Soc. Chim. [3] 1905, 33, 1137-9.	
VARIABLES:	PREPARED BY:	
T/K = 290.8 - 294.8 p/kPa = 100.4 - 100.9	H. L. Clever	

EXPERIMENTAL VALUES:

Temper	ature	Pressure ^a	Solubility
t/°C	<i>T</i> /K	p/mmHg	Volume propane/100 Volumes Solvent
Water;	H ₂ O;	[7732-18-5]	
17.8	291.0	753	6.5
Benzen	e; C ₆ H ₆	0; [71-43-2]	
21.5	294.7	757	1452
Ethano	1; C ₂ H ₆	0; [64-17-5]	
16.6	290.8	754	790
1,1'-0	xybiset	hane or dieth	ylether; C ₄ H ₁₀ O; [60-29-7]
16.6	290.8	757	926
Chloro	form or	trichloromet	hane; CHCl ₃ ; [67-66-3]
21.6	294.8	757	1299
Oil of	turpen	tine	
17.7	290.9	757	1587

Not clear whether this is total pressure or propane partial pressure. It is probably total pressure.

METHOD/APPARATUS/PROCEDURE: Details not given. The data are reported in both papers. SOURCE AND PURITY OF MATERIALS: (1) Propane. Prepared by author from carefully purified propyl iodide by reaction with sodium in liquid ammonia. Melting point/°C = -195 Boiling point/°C = -44.5 Critical temperature/°C = 102. (2) Solvents. No information. ESTIMATED ERROR:

COMPONENTS: (1) Propane; C₃H₈; [74-98-6] (2) 1,2-Ethanediol (Ethylene glycol); J. Chem. Eng. Data, 1971, 16, 340-2. [107-21-1] VARIABLES: T/K: 298 P/kPa: 101.3 PREPARED BY: C. L. Young

T/K	Henry's constant HC3H8/atm	Mole fraction at 1 atm* x C $_{3}$ H $_{8}$
298	409	0.00244

* Calculated by compiler assuming a linear function of $p_{C_3H_8}$ vs $x_{C_3H_8}$ /i.e., $x_{C_3H_8}$ (1 atm) = $1/H_{C_3H_8}$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A conventional gas-liquid chromatographic unit fitted with a thermal conductivity detector was used. The carrier gas was helium. The value of Henry's law constant was calculated from the retention time. The value applies to very low partial pressures of gas and there may be a substantial difference from that measured at latm. pressure. There is also considerable uncertainty in the value of Henry's constant since surface adsorption was not allowed for although its possible existence was noted.

SOURCE AND PURITY OF MATERIALS:

- (1) L'Air Liquide sample; minimum purity 99.9 mole per cent.
- (2) Touzart and Matignon or Serlabo sample; purity 99 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$; $\delta H/atm = \pm 6\%$ (estimated by compiler).

COMPONENTS: (1) Propane; C₃H₈; [74-98-6] Kretschmer, C.B.; Wiebe, R. (2) 2-Propanol; C₃H₈O; [67-63-0] J. Am. Chem. Soc. 1952, 74, 1276-7. VARIABLES: T/K = 273.15-323.15 P/kPa = 67.71-101.39 PREPARED BY: H.L. Clever W. Hayduk

EXPERIMENTAL VALUES	RIMENTAL	VALUES:
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<i>T/</i> K		essure um Hg Partial ²	Mole Fraction ^{1,2}	Ostwald Coefficient ² L/cm ³ cm ⁻³	Bunsen Coefficient ² α/cm^3 (STP) cm ⁻³ atm ⁻¹
273.15	754.9	747.1 760.0	0.05804	18.4	18.4
298.15	507.9 626.7	463.5 582.6	0.0390 0.01830 0.02317	10.4	10.4
	760.5	716.6 760.0	0.02783 0.0295	9.52	8.68
323.15	754.7	577.8 760.0	0.01423 0.0187	6.31	5.29

¹Original data.

Mole fractions at 101.325 kPa were used to determine the following equation for $\ln x_1$ and table of smoothed values:

 $\ln x_1 = 20.274 \ln T + 8044.04/T - 146.016$ Correlation coeff. = 0.9999.

<i>T</i> /K	x_1	T/K	x ₁	
273.15	0.0591	303.15	0.0265	
283.15	0.0433	313.15	0.0219	
193.15	0.0332	323.15	0.0187	

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus was an all glass system which consisted of a monometer, gas handling system, gas buret and solubility bulb equipped with a magnetic stirrer.

The solubility bulb was evacuated and weighed. About 15 cm³ of solvent was distilled into the bulb, the solvent degassed and the bulb reweighed.

A sample of hydrocarbon was condensed into a calibrated tube; it was vaporized into a known volume and the pressure measured. Equilibrium was established between the gas and the solvent. Pressure was again measured.

A detailed description of the apparatus and values of the gas molal volume and 2nd virial coefficient are in (1).

SOURCE AND PURITY OF MATERIALS:

- (1) Philipps Petroleum Co.,
 Research Grade. Specified 99.99
 mole percent pure. Treated to
 remove dissolved gases and
 moisture
- (2) Source not given. Fractionated through a 50-plate column, dried with Mg, stored in a sealed container. Density at 25°C 0.78081 g cm⁻³.

ESTIMATED ERROR:

 $\delta T/K = 0.005$ $\delta p/mm Hg = 0.05$ $\delta x_1/x_1 = 0.005$ (compilers)

REFERENCES:

Kretschmer, C.B.; Wiebe, R.
 J. Am. Chem. Soc. <u>1951</u>, 73, 3778.

²Calculations for 101.325 kPa (760 mm) were by compilers assuming Henry's law, and Raoult's law for solvent partial pressure.

COMPONENTS:

- (1) Propane; C₃H₉; [74-98-6]
- (2) 2-Ethoxyethanol (Ethylcellosolve); $C_4H_{10}O_2$; [110-80-5]

ORIGINAL MEASUREMENTS:

Ezheleva, A.E.; Zorin, A.D.

Tr. Khim. Khim. Tech. (Gorkii) 1961, 1, 37-40.

VARIABLES:

T/K: 303.15-343.15

P/kPa: 101.325 and above

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

<i>T/</i> K	Ostwald Coefficient ² L/cm ³ cm ⁻³	Bunsen Coefficient ² α/cm ³ (STP) cm ⁻³ atm ⁻¹	Mole Fraction ¹	
303.15	10.80	9.67	0.042 (0.0419)3	
313.15	8.98	7.78	0.035 (0.0342)	
323.15	6.98	5.85	0.0274(0.0267)	
333.15	4.94	4.01	0.0196(0.0200)	
343.15	3.60	2.83	0.0145(0.0145)	

Original data given as the inverse of Henry's constant which is equivalent to mole fraction at a gas partial pressure of 101.325 kPa.

$$\ln x_1 = 391.17 - 59.530 \ln T - 16423/T$$

Correlation coefficient = 0.9988

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of a two-chamber, rocking device with separate gas and liquid chambers joined by two tubes and microvalves. The gas chamber was equipped with a pressure gauge. After evacuation, gas and deaerated solvent were separately charged, and then contacted by opening the microvalves and by rocking. The solubility was calculated from a knowledge of the volume of the solvent charged, and the initial and final gas pressures.

The solvent was considered non-volatile and the gas pressure was considered to be the total pressure.

SOURCE AND PURITY OF MATERIALS:

- Source and purity not given. Gas purified by low temperature fractionation and analyzed by gas chromatography.
- Source and purity not given. Refractive index measured:

$$n_D^{20} = 1.4078$$

ESTIMATED ERROR:

 $\delta T/K = 0.05$

$$\delta x_1/x_1 = 0.05$$

(estimated by compiler)

²Ostwald and Bunsen coefficients calculated by compiler using authors' assumption that solvent is non-volatile.

³From equation of smoothed data:

COMPONENTS:

- (1) Propane; C_3H_8 ; [74-98-6]
- (2) 1-Butanol; C₄H₁₀O; [71-36-3]

ORIGINAL MEASUREMENTS:

Hayduk, W.; Castañeda, R.

Can. J. Chem. Eng. 1973, 51, 353-358.

VARIABLES:

T/K: 273.15-323.15

P/kPa: 101.325

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

т/к	Ostwald Coefficient ¹ L/cm ³ cm ⁻³	Bunsen Coefficient ² α/cm (STP) cm^{-3} atm ⁻¹	Mole Fraction ¹
273.15	18.60	18.60	0.0706 (0.0706) ³ 0.0367 (0.0367) 0.0226 (0.0226)
298.15	10.07	9.23	
323.15	6.43	5.44	

- 1 Original data.
- ² Calculated by compiler.
- The mole fraction solubility of the original data was used to determine the following equations for ΔG° and $\ln x_1$ and table of smoothed values: $\Delta G^{\circ}/J \text{ mol}^{-1} = -RT \ln x_1 = 669.59 \text{ } T 87.560 \text{ } T \ln T 42705$

 $\ln x_1 = 5136.5/T + 10.5316 \ln T - 80.538$

Std. deviation for $\Delta G^{\circ} = 0.6 \text{ J mol}^{-1}$

<i>T/</i> K	ΔG°/J mol ⁻¹		<i>T</i> /K	ΔG°/J mol ⁻¹	x_1
273.15 283.15 293.15 298.15	6019 6911 7772 8192	0.0706 0.0531 0.0412 0.0367	303.15 313.15 323.15	8604 9406 10181	0.0329 0.0270 0.0226

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A volumetric method using a glass apparatus was employed. Degassed solvent contacted the gas while flowing as a thin film, at a constant rate, through an absorption spiral into a solution buret. A constant solvent flow was obtained by means of a calibrated syringe pump. The solution at the end of the spiral was considered saturated. Dry gas was maintained at atmospheric pressure in a gas buret by mechanically raising the mercury level in the buret at an adjustable The solubility was calculated rate. from the constant slope of volume of gas dissolved and volume of solvent injected.

Degassing was accomplished using a two stage vacuum process described by Clever et al. (1).

SOURCE AND PURITY OF MATERIALS:

- Matheson Co. Specified as instrument grade of minimum purity 99.5 per cent.
- Fisher Scientific. Specified minimum purity 99.0 per cent.

ESTIMATED ERROR:

$$\delta T/K = 0.1$$

$$\delta x_{7}/x_{7} = 0.01$$

REFERENCES:

 Clever, H.L.; Battino, R.; Saylor, J.H.; Gross, P.M.
 J. Phys. Chem. 1971, 61, 1078.

COMPONENTS:

- (1) Propane; C₃H₈; [74-98-6]
- (2) 3-Methyl-1-butanol; C₅H₁₂O; [123-51-3]

ORIGINAL MEASUREMENTS:

Friedel, C.; Gorgeu, A.

Compt. rendu 1908, 127, 590-4.

VARIABLES:

T/K = 289, 296p/kPa = 100.0, 101.3 PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

Temper	ature	Pressure	Solubility
t/°C	T/K	p/m Hg	Volume Propane/ Volume Alcohol
16	289	0.750	12
23	296	0.760	11

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In the original paper the alcohol was named simply amyl alcohol. However, the boiling point corresponds to the alcohol later named primary isoamyl alcohol or 3-methyl-l-butanol.

SOURCE AND PURITY OF MATERIALS:

- (1) Propane. Prepared by authors from isopropyl iodide and zinc plus a small amount of hydrochloric acid.
- (2) 3-Methyl-1-butanol. Prepared by the authors. Boiling point 130-132 °C.

ESTIMATED ERROR:

			71100				
COMPONENTS	3:			ORIGINAL MEASUREMENTS:			
<pre>(1) Propane; C₃H₈; [74-98-6] (2) 1-Heptanol; C₇H₁₆O; [111-70-6]</pre>				Dim, A.; Gardner, G.R.; Ponter, A.B.; Wood, T. J. Chem. Eng. Japan 1971, 4, 92-95			
VARIABLES	<i>T</i> /K:	298.15 101.325		PREPARED BY: W. Hayduk			
EXPERIMEN:	TAL VALU	ES:					
T/K		rility ¹ ⁵ (mol cm ⁻³)	Ostwald Coefficie L/cm ³ cm ⁻³	ent²	Bunsen Coefficient ² α/cm ³ (STP) cm ⁻³ atm ⁻¹	Mole Fraction ²	
298.15		40.8	9.82		8.95	0.0546	

MEMUOD /AD	DADATUC	/PROCEDURE:	AUXILIARY	,	ATION AND PURITY OF MATE	DTATC.	
	√ailabl				available.	ninus.	
				δο 1	ATED ERROR: /c ₁ = 0.03 (comp	iler)	
				REFER	ENCES:		

Alco	phols 34
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propane; C ₃ H ₈ ; [74-98-6]	Lenoir, J-Y.; Renault, P.; Renon, H.
(2) Benzenemethanol, (Benzyl alcohol); C ₇ H ₈ O; [100-51-6]	J. Chem. Eng. Data, <u>1971</u> , 16, 340-2
VARIABLES:	PREPARED BY:
T/K: 298 P/kPa: 101.3	C. L. Young
XPERIMENTAL VALUES:	
T/K Henry's constar	Mole fraction at 1 atm* ${}^x\mathrm{C}_3\mathrm{H}_8$
298 50.8	0.0197
* Calculated by compiler assuming a lie., $x_{C_3H_8}$ (1 atm) = $1/H_{C_3H_8}$	Linear function of $p_{C_3H_8}$ vs $x_{C_3H_8}$,
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A conventional gas-liquid chromato- graphic unit fitted with a thermal	(1) L'Air Liquide sample; minimum purity 99.9 mole per cent.
conductivity detector was used. The carrier gas was helium. The value of Henry's law constant was calculated from the retention time. The value	(2) Touzart and Matignon or Serlabo sample; purity 99 mole per cent.

A conventional gas-liquid chromatographic unit fitted with a thermal conductivity detector was used. The carrier gas was helium. The value of Henry's law constant was calculated from the retention time. The value applies to very low partial pressures of gas and there may be a substantial difference from that measured at l atm. pressure. There is also considerable uncertainty in the value of Henry's constant since surface adsorption was not allowed for although its possible existence was noted.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$; $\delta H/atm = \pm 6$ % (estimated by compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propane; C ₃ H ₈ ; [74-98-6] (2) Phenol; C ₆ H ₆ O; [108-95-2]	Lenoir, J-Y.; Renault, P.; Renon, H. J. Chem. Eng. Data, 1971, 16, 340-3
VARIABLES: T/K: 323.2 P/kPa: 101.3	PREPARED BY: C. L. Young

EXPERIMENTAL VALUES:

 		Mole fraction at 1 atm*
T/K	Henry's constant HC3H8/atm	C ₃ H ₈
222.2	101	0.00990
323.2	101	0.00990

* Calculated by compiler assuming a linear function of $p_{C_3H_8}$ vs $x_{C_3H_8}$ i.e., $x_{C_3H_8}$ (1 atm) = $1/H_{C_3H_8}$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A conventional gas-liquid chromatographic unit fitted with a thermal conductivity detector was used. The carrier gas was helium. The value of Henry's law constant was calculated from the retention time. The value applies to very low partial pressures of gas and there may be a substantial difference from that measured at l atm. pressure. There is also considerable uncertainty in the value of Henry's constant since surface adsorption was not allowed for although its possible existence was noted.

SOURCE AND PURITY OF MATERIALS:

- (1) L'Air Liquide sample; minimum purity 99.9 mole per cent.
- (2) Touzart and Matignon or Serlabo sample; purity 99 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$; $\delta H/atm = \pm 6\%$ (estimated by compiler).

COMPONENTS: (1) Propane; C₃H₈; [74-98-6] Gerrard, W. (2) Benzenemethanol (Benzyl alcohol); J. Appl. Chem. Biotechnol. C₇H₈O; [100-51-6] 1973, 23, 1-17. VARIABLES: T/K: 273.2-298.2 P/kPa: 101.3 CRIGINAL MEASUREMENTS: Gerrard, W. J. Appl. Chem. Biotechnol. 1973, 23, 1-17.

EXPERIMENTAL VALUES:

Total pressure = 101.3 kPa

r/k	Mole ratio	Mole fraction of propane #	
273.2	0.039	0.038	
278.2	0.0339	0.0328	
283.2	0.0296	0.0287	
293.2	0.0243	0.0237	
298.2	0.0224	0.0219	

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Gas was passed into a known weight of pure liquid in a bubbler tube at a total pressure measured using a manometer assembly. The amount of absorbed gas was estimated by weighing. The temperature was controlled to within 0.2 K. The apparatus and procedure are described by Gerrard, ref. (1).

SOURCE AND PURITY OF MATERIALS:

No details given except that "all compounds were purified by conventional procedures".

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$; $\delta x/x = \pm 3\%$ (estimated by compiler).

REFERENCES:

Gerrard, W.
 J. Appl. Chem. Biotechnol.
 1972, 22, 623.

[#] Calculated by compiler.

			ODTOTNIA IMIANIS		
COMPONENTS:		Į.	ORIGINAL MEASUREMENTS:		
(1) Propane; C ₃ H ₈ ; [74-98-6]			Dim, A.; Gardner, G.R.; Ponter, A.B.; Wood, T.		
(2) 1-Octanol; C ₈ H ₁₈ O; [111-87-5]			J. Chem. Eng. Japan <u>1971</u> , 4, 92-95.		
VARIABLES:			PREPARED BY:		
	T/K: 298.15		W. Hayo	luk	
P/1	kPa: 101.325				
EXPERIMENTAL	VALUES:				
T/K S	olubility ¹ ₁ /10 ⁵ (mol cm ⁻³)	Ostwald Coefficien L/cm ³ cm ⁻³	Bunsen Coefficient ² α/cm ³ (STP) cm ⁻³ atm ⁻¹	Mole Fraction ²	
298.15	40.3	9.70	8.85	0.0602	
¹Original ²Calculat		sing the rea	l gas molar volume	··	
				·	
² Calculat	ed by compiler u		INFORMATION		
² Calculat				MATERIALS:	
² Calculat	ed by compiler us		INFORMATION SOURCE AND PURITY OF	MATERIALS:	
² Calculat	ed by compiler us		INFORMATION SOURCE AND PURITY OF	MATERIALS:	
² Calculat	ed by compiler us		INFORMATION SOURCE AND PURITY OF Not available	MATERIALS:	

EXPERIMENTAL VALUES:

Total pressure = 101.3 kPa

T/K	Mole ratio	Mole fraction of propane #
268.2	0.190	0.160
273.2	0.162	0.139
278.2	0.137	0.120
283.2	0.120	0.107
293.2	0.093	0.0851
298.2	0.086	0.0792

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Gas was passed into a known weight of pure liquid in a bubbler tube at a total pressure measured using a manometer assembly. The amount of absorbed gas was estimated by weighing. The temperature was controlled to within 0.2 K. The apparatus and procedure are described by Gerrard, ref. (1).

SOURCE AND PURITY OF MATERIALS:

No details given except that "all compounds were purified by conventional procedures".

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$; $\delta x/x = \pm 3\%$ (estimated by compiler).

REFERENCES:

Gerrard, W.
 J. Appl. Chem. Biotechnol.
 1972, 22, 623.

[#] Calculated by compiler.

COMPONENTS: (1) Butane; C₄H₁₀; [106-97-8] Kretschmer, C.B.; Wiebe, R. (2) Methanol; CH₄O; [67-56-1] J. Am. Chem. Soc. 1952, 74, 1276-7. VARIABLES: T/K = 298.15-323.15 P/kPa = 65.94-101.59 PREPARED BY: H.L. Clever W. Hayduk

T/K		ssure m Hg	Mole Fraction ^{1,2}	Ostwald Coefficient ²	Bunsen Coefficient ²
	Total 1	Partial ²	/x ₁	L/cm ³ cm ⁻³	α/cm³(STP)cm-³atm-1
298.15	494.6	371.3	0.01651		
	635.6	513.2	0.02410		
	762.0	640.6	0.03171		
		760.0	0.0398	24.1	21.8
308.15	750.6	547.3	0.01920		
		760.0	0.0267	16.4	14.3
323.15	756.8	346.6	0.008075		
		760.0	0.0177	11.1	9.23

¹Original data.

Mole fractions at 101.325 kPa were used to determine the following equation for $\ln\,x_{_{1}}$ and table of smoothed values:

 $\ln x_1 = 75.474 \ln T + 26544/T - 522.274$ Correlation coeff. = 0.9999

	<u> </u>	<i>T</i> /K	x_1
298.15	0.0398	313.15	0.0227
303.15	0.0321	323.15	0.0177

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus was an all glass system which consisted of a monometer, gas handling system, gas buret and solubility bulb equipped with a magnetic stirrer.

The solubility bulb was evacuated and weighed. About 15 cm³ of solvent was distilled into the bulb, the solvent degassed and the bulb reweighed.

A sample of hydrocarbon was condensed into a calibrated tube; it was vaporized into a known volume and the pressure measured. Equilibrium was established between the gas and the solvent. Pressure was again measured.

A detailed description of the apparatus and values of the gas molal volume and 2nd virial coefficient are in (1).

SOURCE AND PURITY OF MATERIALS:

- (1) Phillips Petroleum Co., Research Grade. Specified 99.78 mole percent pure. Treated to remove dissolved gases and moisture.
- (2) Source not given. Treated to remove acetone and aldehydes. Fractionated through a 50-plate column, dried with Mg, stored in a sealed container. Density at 25°C 0.78653 g cm⁻³.

ESTIMATED ERROR:

 $\delta T/K = 0.005$ $\delta p/mm Hg = 0.05$ $\delta x_1/x_1 = 0.005$

REFERENCES:

Kretschmer, C.B.; Wiebe, R.
 J. Am. Chem. Soc. <u>1951</u>, 73, 3778.

²Calculations for 101.325 kPa (760 mm) were by compilers assuming Henry's law, and Raoult's law for solvent partial pressure.

EXPERIMENTAL VALUES:

<i>T/</i> K		essure /mm Hg Partial ²	Mole fraction 1,2	Ostwald Coefficient ² L/cm ³ cm ⁻³	Bunsen Coefficient ² α/cm ³ (STP) cm ⁻³ atm ⁻¹
298.15	238.0 325.8 393.3 436.8 589.9	179.1 267.4 335.3 379.1 533.2	0.01517 0.02334 0.02999 0.03440 0.05144		
308.15	739.5 233.0 330.1 430.5 713.3	683.9 760.0 130.0 227.7 328.9 620.0	0.07092 0.0815 0.008298 0.01484 0.02198 0.04476	35.9	32.5
323.15	337.8 487.5 590.6 733.5	760.0 117.4 268.6 372.8 517.3 760.0	0.0560 0.005210 0.01218 0.01716 0.02442 0.0368	24.6 16.4	13.6

¹Original data.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus was an all-glass system which consisted of a manometer, gas handling system, gas buret and solubility bulb equipped with a magnetic stirrer.

The solubility bulb was evacuated and weighed. About 15 cm³ of solvent was distilled into the bulb, the solvent degassed and the bulb reweighed.

A sample of hydrocarbon was condensed into a calibrated tube; it was vaporized into a known volume and the pressure measured. Equilibrium was established between the gas and the solvent. Pressure was again measured.

SOURCE AND PURITY OF MATERIALS:

- (1) Phillips Petroleum Co. Research grade, 99.78 mole per cent. Removed dissolved air and moisture.
- (2) Commercial absolute alcohol sample fractionated, treated with Mg ethylate, stored in sealed container until used. Density, at 25°C 0.78505 g cm⁻³

ESTIMATED ERROR:

 $\delta T/K = 0.005$ $\delta p/mm Hg = 0.05$ $\delta x_1/x_1 = 0.005 \text{ (compilers)}$

²Calculations for 101.325 kPa (760 mm) were by compilers by extrapolation of data for lower pressures, and by assuming Raoult's law for solvent partial pressure.

continued..

352 **Alcohols** COMPONENTS: ORIGINAL MEASUREMENTS: (1) Butane; C₄H₁₀; [106-97-8] Kretschmer, C.B.; Wiebe, R. (2) Ethanol; C₂H₆O; [64-17-5] J. Am. Chem. Soc. 1951, 73, 3778-81. VARIABLES: PREPARED BY: T/K = 298.15-323.15H.L. Clever P/kPa = 23.88-98.59W. Hayduk EXPERIMENTAL VALUES: concluded Mole fraction solubilities at 101.325 kPa were used to determine the following equation for $\ln x_1$ and table of smoothed values:

 $\ln x_1 = 53.1055 \ln T + 19544.3/T - 370.633$

Correlation coefficient = 0.9999

<i>T/</i> K	x_1	<i>T</i> /K	<u> </u>
298.15	0.0815	313.15	0.0478
303.15	0.0668	323.15	0.0368
308.15	0.0560		

AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: ESTIMATED ERROR: REFERENCES:

COMPONENTS: (1) Butane; C₄H₁₀; [106-97-8] (2) Water; H₂O; [7732-18-5] Ethanol; C₂H₆O; [64-17-5] Diethylether; C₄H₁₀O; [60-29-7] Chloroform; CHCl₃; [67-66-3] VARIABLES: T/K = 290, 291 p/kPa = 102.9 - 104.8 ORIGINAL MEASUREMENTS: Lebeau, P. Bull. Acad. Roy. Belg. 1908, 300-4. PREPARED BY: H. L. Clever

EXPERIMENTAL VALUES:

Tempera	emperature Pressure ^a		Solubility		
t/°C	T/K	p/mmHg	Volume Butane/Volume Solvent		
Water		· · · · · · · · · · · · · · · · · · ·			
17	290	772	0.15		
Ethanol					
17	290	775	18.83		
Diethyl	ether	or 1'1'-oxyb	isethane		
18	291	773	29.8		
Chlorof	orm or	trichlorome	thane		
17	290	786	32.5		

Not clear whether this is total pressure or butane partial pressure. It is probably the total pressure.

AU	JXILIARY INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Details not given.	(1) Butane. Prepared by author by the reaction of sodium in liquid ammonia on butyl iodide. The normal boiling point is 0.5 °C, and the critical temperature is 151-2 °C.
	(2) Solvents. No information.
	ESTIMATED ERROR:
	JOINING BRACK
	REFERENCES:

ATTYTITADY INCODMATION

ORIGINAL MEASUREMENTS: COMPONENTS: (1) Butane; C₄H₁₀; [106-97-8] Gerrard, W. (2) 1,2-Ethanediol (ethylene glycol); J. Appl. Chem. Biotechnol. [107-21-1] C2H6O2; 1973, 23, 1-17. or 1,2,3-Propanetriol (glycerol); $C_3H_8O_3$; [56-81-5] VARIABLES: PREPARED BY: T/K: 275.2 C. L. Young P/kPa: 101.3 EXPERIMENTAL VALUES:

Total pressure = 101.3 kPa

T/K	p/mmHg	Mole ratio	Mole fraction of butane [#]	
	1,2-Eth	anediol; C ₂ H ₆ O ₂	; [107-21-1]	
275.2	742	0.0598	0.0564	
	1,2,3-P	ropanetriol; C ₃	H ₈ O ₃ ; [56-81-5]	
275.2	742	0.010	0.0099	

AUXILIARY INFORMATION

Gas was passed into a known weight of pure liquid in a bubbler tube at a total pressure measured using a manometer assembly. The amount of absorbed gas was estimated by weighing. The temperature was controlled to within 0.2 K. The apparatus and procedure are described by Gerrard, ref. (1).

METHOD /APPARATUS / PROCEDURE:

SOURCE AND PURITY OF MATERIALS:

No details given except that "all compounds were purified by conventional procedures".

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$; $\delta x/x = \pm 3\%$ (estimated by compiler).

REFERENCES:

1. Gerrard, W. J. Appl. Chem. Biotechnol. 1972, 22, 623.

Calculated by compiler.

COMPONENTS:

- (1) Butane; C₄H₁₀; [106-97-8]
- (2) Ethanol; C₂H₆O; [64-17-5]

ORIGINAL MEASUREMENTS:

Frankland, E.

J. Chem. Soc. 1849, 2, 263-96.

Liebig's Ann. 1849, 71, 171-213.

VARIABLES:

T/K = 287.4 $p_1/kPa = 99.3$ PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

Temperature	Pressure	Solubility, Volume gas/
$t/^{0}$ C T/K	p_1/mmHg	volume alcohol
14.2 287.4	744.8	18.13

The author states that most of the gas is evolved from the alcohol on the addition of a small amount of water.

The author also describes an experiment in which 1 volume of ethanol takes up 1.22 volumes of ethane at 8.8 $^{\circ}$ C (282.0 K) at a pressure of 665.5 mmHg (88.7 kPa).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Eudiometer. The dry gas was treated with sulfuric acid before the solubility experiment.

SOURCE AND PURITY OF MATERIALS:

- (1) Butane. Prepared by the reaction of ethyl iodide with zinc at $150~^{\circ}\mathrm{C}$.
- (2) Ethanol. Described as freshly boiled absolute ethanol.

ESTIMATED ERROR:

COMPONENTS:

(1) Butane; C₄H₁₀; [106-97-8]

(2) 2-Propanol; C₃H₉O; [67-63-0]

ORIGINAL MEASUREMENTS:

Kretschmer, C.B.; Wiebe, R.

J. Am. Chem. Soc. 1952, 74, 1276-7.

VARIABLES:

T/K = 298.15-323.15

P/kPa = 57.36-101.36

PREPARED BY:

H.L. Clever

W. Hayduk

EXPERIMENTAL VALUES:

T/K	p/m	ssure m Hg	Mole Fraction ^{1,2}	Ostwald Coefficient ²	Bunsen Coefficient ²
	Total 1	Partial ²	/x ₁	L/cm³cm-3	α/cm³(STP)cm-³atm-1
298.15	430.2	387.4	0.05285		
	479.5	537.8	0.07755		
	752.7	712.5	0.11056		
		760.0	0.1179	41.2	38.2
308.15	760.3	685.4	0.07531		
		760.0	0.0835	28.8	25.2
323.15	752.1	580.1	0.04149		
		760.0	0.0544	18.8	15.6

¹Original data.

Mole fractions at 101.325 kPa were used to determine the following equation for $\ln\ x_1$ and table of smoothed values:

 $\ln x$, = 26.142 $\ln T$ + 11093.4/T - 188.292 Correlation coeff. = 0.9999.

	_
313.15 0.0716	6
323.15 0.054	4

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus was an all glass system which consisted of a monometer, gas handling system, gas buret and solubility bulb equipped with a magnetic stirrer.

The solubility bulb was evacuated and weighed. About 15 cm³ of solvent was distilled into the bulb, the solvent degassed and the bulb reweighed.

A sample of hydrocarbon was condensed into a calibrated tube; it was vaporized into a known volume and the pressure measured. Equilibrium was established between the gas and the solvent. Pressure was again measured.

A detailed description of the apparatus and values of the gas molal volume and 2nd virial coefficient are in (1).

SOURCE AND PURITY OF MATERIALS:

- (1) Phillips Petroleum Co.,
 Research Grade. Specified 99.78
 mole percent pure. Treated to
 remove dissolved gases and
 moisture.
- (2) Source not given. Fractionated through a 50-plate column, dried with Mg, stored in a sealed container. Density at 25°C 0.78081 g cm⁻³.

ESTIMATED ERROR:

 $\delta T/K = 0.005$

 $\delta p/\text{mm} \text{ Hg} = 0.05$

 $\delta x_1/x_1 = 0.005$ (compilers)

- 1. Kretschmer, C.B.; Wiebe, R.
 - J. Am. Chem. Soc. 1951, 73, 3778.

²Calculations for 101.325 kPa (760 mm) were by compilers assuming Henry's law, and Raoult's law for solvent partial pressure.

COMPONENTS:

- (1) Butane; C_4H_{10} ; [106-97-8]
- (2) 1-Butanol; C₄H₁₀0; [71-36-3]

ORIGINAL MEASUREMENTS:

Hayduk, W.; Castañeda, R.

Can. J. Chem. Eng. <u>1973</u>, 51, 353-358.

VARIABLES:

T/K: 278.15-323.15

P/kPa: 101.325

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

<i>T</i> /K	Ostwald Coefficient ¹ L/cm ³ cm ⁻³	Bunsen Coefficient ² α/cm ³ (STP)cm ⁻³ atm ⁻¹	Mole Fraction ¹
278.15	157.4	154.6	0.393 (0.393) ³ 0.141 (0.141) 0.0686 (0.0687)
298.15	42.4	38.8	
323.15	20.3	17.2	

- 1 Original data.
- ² Calculated by compiler.
- 3 The mole fraction solubility of the original data was used to determine the following equations for $\Delta {\rm G}^{\circ}$ and $\ln\,x_{\,1}^{}$ and table of smoothed values:

 $\Delta G^{\circ}/J \text{ mol}^{-1} = -RT \ln x_1 = 3788.47 T - 548.330 T \ln T - 193210$ $\ln x_1 = 23238.9/T + 65.9526 \ln T - 455.674$

Std. deviation for $\Delta G^{\circ} = 2.4 \text{ J mol}^{-1}$

<i>T</i> /K	ΔG°/J mol-1	<u> </u>		ΔG°/J mol-1	<u>x</u> 1
278.15	2159.5	0.3929	303.15	5412.4	0.1167
283.15	2905.3	0.2910	313.15	6391.2	0.0858
293.15	4252.1	0.1746	323.15	7195.5	0.0687
298.15	4855.3	0.1410			

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A volumetric method using a glass apparatus was employed. Degassed solvent contacted the gas while flowing as a thin film, at a constant rate, through an absorption spiral into a solution buret. A constant solvent flow was obtained by means of a calibrated syringe pump. The solution at the end of the spiral was considered saturated. Dry gas was maintained at atmospheric pressure in a gas buret by mechanically raising the mercury level in the buret at an adjustable The solubility was calculated from the constant slope of volume of gas dissolved and volume of solvent injected.

Degassing was accomplished using a two stage vacuum process described by Clever et al. (1).

SOURCE AND PURITY OF MATERIALS:

- Matheson Co. Specified as instrument grade of purity 99.5 per cent.
- Fisher Scientific. Specified minimum purity 99.0 per cent.

ESTIMATED ERROR:

 $\delta T/K = 0.1$

 $\delta x_1/x_1 = 0.01$

REFERENCES:

 Clever, H.L.; Battino, R.; Saylor, J.H.; Gross, P.M.
 J. Phys. Chem. 1971, 61, 1078.

COMPONENTS:

- (1) Butane; C₄H₁₀; [106-97-8]
- (2) 1-Butanol; C₄H₁₀O; [71-36-3]

ORIGINAL MEASUREMENTS:

Blais, C.; Hayduk, W.

J. Chem. Eng. Data 1983, 28, 181-184.

VARIABLES:

T/K: 298.15,323.15

P/kPa: 101.325

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

<i>T</i> /K	Ostwald Coefficient ¹ L/cm ³ cm ⁻³	Bunsen Coefficient ² α/cm ³ (STP)cm ⁻³ atm ⁻¹	Mole Fraction ¹
298.15	41.6	38.11	0.139 (0.1390) ³ 0.0725(0.0725)
323.15	21.5	18.17	

¹Original data.

$$\Delta G^{\circ}/J \text{ mol}^{-1} = -RT \text{ ln } x_1 = 663.30 T \text{ ln } T - 3617.3 T$$

$$\ln x_1 = 44.0836 - 8.08356 \ln T$$

<i>T</i> /K	10-4ΔG°/J mol-1	x
298.15	4.828	0.1390
303.15	5.243	0.1215
313.15	6.090	0.0935
323.15	6.958	0.0725

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A volumetric method using a glass apparatus was employed. Degassed solvent contacted the gas while flowing as a thin film, at a constant rate, through an absorption spiral into a solution buret. A constant solvent flow was obtained by means of a calibrated syringe pump. The solution at the end of the spiral was considered saturated. Dry gas was maintained at atmospheric pressure in a gas buret by mechanically raising the mercury level in the buret at an adjustable rate. The solubility was calculated from the constant slope of volume of gas dissolved and volume of solvent injected.

Degassing was accomplished using a two stage vacuum process described by Clever et al. (1).

SOURCE AND PURITY OF MATERIALS:

- Liquid Carbonic. Pure grade of minimum purity 99.0 per cent.
- Canlab (J.T. Baker Company). Spectrophotometric grade of minimum specified purity 99.5 per cent.

ESTIMATED ERROR:

 $\delta T/K = 0.1$

 $\delta x_1/x_1 = 0.01$

REFERENCES:

 Clever, H.L.; Battino, R.; Saylor, J.H.; Gross, P.M.
 J. Phys. Chem. 1957, 61, 1079

²Calculated by compiler.

 $^{^3}$ The mole fraction solubility of the original data was used to determine the following equations for ΔG° and $\ln~x_1$ and table of smoothed values:

COMPONENTS:

- (1) Butane; C₄H₁₀; [106-97-8]
- (2) 3-Methyl-1-butanol; C₅H₁₂O; [123-51-3]

ORIGINAL MEASUREMENTS:

Friedel, C.; Gorgeu, A.

Compt. rendu 1908, 127, 590-4.

VARIABLES:

PREPARED BY:

T/K = 286, 295p/kPa = 98.7, 101.3 H. L. Clever

EXPERIMENTAL VALUES:

Temper	ature	Pressure	Solubility
t/°C	T/K	p/mHg	Volume Butane/ Volume Alcohol
13	286	0.740	72
22	295	0.760	44

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In the original paper the alcohol was named simply amyl alcohol. However the boiling point corresponds to the alcohol later named primary iso amyl alcohol or 3-methyl-l-butanol.

SOURCE AND PURITY OF MATERIALS:

- Butane. Prepared by authors from sec-butyl iodide, zinc and hydrochloric acid.
- (2) 3-Methyl-1-butanol. Prepared by the authors. Boiling point 130-132 °C.

ESTIMATED ERROR:

COMPONENTS:

(1) Butane; C₄H₁₀; [106-97-8]

Lenoir, J-Y.; Renault, P.; Renon, H.

(2) Phenol; C₆H₆O; [108-95-2]

VARIABLES:

T/K: 323.2

P/kPa: 101.3

CRIGINAL MEASUREMENTS:

Lenoir, J-Y.; Renault, P.; Renon, H.

J. Chem. Eng. Data, 1971, 16, 340-2.

Alcohols

EXPERIMENTAL VALUES:

T/K	Henry's constant HC4H10	Mole fraction at 1 atm* ${}^{x}C_{4}H_{10}$
323.2	37.5	0.0267

* Calculated by compiler assuming a linear function of $p_{C_4H_{10}}$ vs $x_{C_4H_{10}}$, i.e., $x_{C_4H_{10}}$ (1 atm) = $1/H_{C_4H_{10}}$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A conventional gas-liquid chromatographic unit fitted with a thermal conductivity detector was used. The carrier gas was helium. The value of Henry's law constant was calculated from the retention time. The value applies to very low partial pressures of gas and there may be a substantial difference from that measured at l atm. pressure. There is also considerable uncertainty in the value of Henry's constant since surface adsorption was not allowed for although its possible existence was noted.

SOURCE AND PURITY OF MATERIALS:

- (1) L'Air Liquide sample; minimum purity 99.9 mole per cent.
- (2) Touzart and Matignon or Serlabo sample; purity 99 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$; $\delta H/atm = \pm 6$ % (estimated by compiler).

Alcohols 361 ORIGINAL MEASUREMENTS: COMPONENTS: (1) Butane; C4H10; [106-97-8] Lenoir, J-Y.; Renault, P. Renon, H. (2) Benzenemethanol, (Benzyl alcohol); J. Chem. Eng. Data 1971, 16, 340-2 C₇H₈O; [100-51-6] **VARIABLES:** PREPARED BY: 298.15 T/K: C.L. Young P/kPa: 101.3 EXPERIMENTAL VALUES: Mole fraction at 1 atm* Henry's Constant T/K H_{C4H10}/atm xC4H10 15.7 0.0637 298.15 Calculated by compiler assuming a linear function of $p_{C_hH_{10}}$ vs $x_{C_hH_{10}}$, ie., $x_{C_4H_{10}}$ (1 atm) = $1/H_{C_4H_{10}}$ AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS:

A conventional gas-liquid chromatographic unit fitted with a thermal conductivity detector was used. The carrier gas was helium. The value of Henry's law constant was calculated from the retention time. The value applies to very low partial pressures of gas and there may be a substantial difference from that measured at latm. pressure. There is also considerable uncertainty in the value of Henry's constant since surface adsorption was not allowed for although its possible existence was noted.

- (1) L'Air Liquide sample; minimum purity 99.9 mole per cent.
- (2) Touzart and Matignon or Serlabo sample; purity 99 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$; $\delta H/atm = \pm 6\%$ (estimated by compiler).

EXPERIMENTAL VALUES:

Total pressure = 101.3 kPa

T/K	Mole ratio	Mole fraction of butane [#]
278.2	1.78	0.640
283.2	0.702	0.412
293.2	0.400	0.286

AUXILIARY INFORMATION

METHOD APPARATUS/PROCEDURE:

Gas was passed into a known weight of pure liquid in a bubbler tube at a total pressure measured using a manometer assembly. The amount of absorbed gas was estimated by weighing. The temperature was controlled to within 0.2 K. The apparatus and procedure are described by Gerrard, ref. (1).

SOURCE AND PURITY OF MATERIALS:

No details given except that "all compounds were purified by conventional procedures".

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1;$ $\delta x/x = \pm 3\%$ (estimated by compiler).

REFERENCES:

Gerrard, W.
 J. Appl. Chem. Biotechnol.
 1972, 22, 623.

[#] Calculated by compiler.

COMPONENTS:

- (1) 2-Methylpropane (isobutane); C_4H_{10} ; [75-28-5]
- (2) Methanol; CH₄O; [67-56-1]

ORIGINAL MEASUREMENTS:

Kretschmer, C.B.; Wiebe, R.

J. Am. Chem. Soc. 1952, 74, 1276-7.

VARIABLES:

T/K = 298.15-323.15

P/kPa = 48.53-101.9

PREPARED BY:

H.L. Clever W. Hayduk

EXPERIMENTAL VALUES:

T/K	_	essure nm Hg Partial ²	Mole Fraction 1,2 /x ₁	Ostwald Coefficient ² L/cm ³ cm ⁻³	Bunsen Coefficient ² α/cm³(STP)cm-³atm-1
298.15	364.0 548.2 764.3	293.5 424.5 641.5	0.00710 0.01316 0.02103	15.3	12.0
308.15	757.7	760.0 553.2 760.0	0.0256 0.01370 0.0188	11.4	13.9
323.15	758.1	347.1 760.0	0.00600 0.01314	8.22	6.82

10riginal data.

²Calculations for 101.325 kPa (760 mm) were by compilers assuming Henry's law, and Raoult's law for solvent partial pressure.

Mole fractions at 101.325 kPa were used to determine the following equation for $\ln\,x_1$ and table of smoothed values:

 $\ln x_1 = 36.912 \ln T + 14,025/T - 261.016$ Correlation coeff. = 0.9999.

<i>T</i> /K	x	<i>T</i> /K	x
298.15	0.0256	313.15	0.0165
303.15	0.0218	323.15	0.0131

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus was an all glass system which consisted of a monometer, gas handling system, gas buret and solubility bulb equipped with a magnetic stirrer.

The solubility bulb was evacuated and weighed. About 15 cm³ of solvent was distilled into the bulb, the solvent degassed and the bulb reweighed.

A sample of hydrocarbon was condensed into a calibrated tube; it was vaporized into a known volume and the pressure measured. Equilibrium was established between the gas and the solvent. Pressure was again measured.

A detailed description of the apparatus and values of the gas molal volume and 2nd virial coefficient are in (1).

SOURCE AND PURITY OF MATERIALS:

- (1) Phillips Petroleum Co.,
 Research Grade. Specified 99.88
 mole percent pure. Treated to
 remove dissolved gases and
 moisture.
- (2) Source not given. Treated to remove acetone and aldehydes. Fractionated through a 50-plate column, dried with Mg, stored in a sealed container. Density at 25°C 0.78653 g cm⁻³.

ESTIMATED ERROR:

 $\delta T/K = 0.005$

 $\delta p/\text{mm}$ Hg = 0.05

 $\delta x_1/x_1 = 0.005$ (compilers)

REFERENCES:

Kretschmer, C.B.; Wiebe, R.
 J. Am. Chem. Soc. 1951, 73, 3778.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methylpropane (isobutane); C ₄ H ₁₀ ; [75-28-5] (2) Ethanol; C ₂ H ₆ O; [64-17-5]	Kretschmer, C.B.; Wiebe, R. J. Am. Chem. Soc. 1951, 73, 3778-81.
VARIABLES: T/K = 283.15-323.15 P/kPa = 30.25-101.38	PREPARED BY: H.L. Clever W. Hayduk

EXPERIMENTAL VALUES: concluded

Mole fraction solubilities at 101.325 kPa (760 mm) were used to determine the following equation for $\ln x_1$ and table of smoothed values:

 $\ln x_1 = 18.020 \ln T + 8122.2/T - 132.89$ Correlation coeff. = 0.9999.

<i>T</i> /K	<u> </u>	<i>T/</i> K	x_1
283.15	0.0851	303.15	0.0439
293.15	0.0598	313.15	0.0335
298.15	0.0509	323.15	0.0264

AUXILIARY INFORMATION

THOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
	ESTIMATED ERROR:
	REFERENCES:
	REFERENCES:

COMPONENTS:

- (1) 2-Methylpropane (isobutane); C₄H₁₀; [75-28-5]
- (2) Ethanol; C₂H₆O; [64-17-5]

ORIGINAL MEASUREMENTS:

Kretschmer, C.B.; Wiebe, R.

J. Am. Chem. Soc. 1951, 73, 3778-81.

VARIABLES:

T/K = 283.15-323.15

P/kPa = 30.25-101.38

PREPARED BY:

H.L. Clever

W. Hayduk

EXPERIMENTAL VALUES:

<i>T</i> /K		essure /mm Hg Partial²	Mole Fraction 1,2 /x ₁	Ostwald Coefficient ² L/cm ³ cm ⁻³	Bunsen Coefficient ² α/cm ³ (STP) cm ⁻³ atm ⁻¹
283.15	389.7 549.6	366.6 526.9 760.0	0.03528 0.05443 0.0852	36.2	34.7
298.15	226.9 305.8 439.5 725.4	167.7 246.9 381.1 668.2	0.009739 0.01454 0.02316 0.04368		
308.15	313.1 455.2 602.4	760.0 210.2 353.0 501.0	0.0512 0.00955 0.01643 0.02391	21.8	19.8
323.15	760.4 317.3 542.3	659.9 760.0 96.4 323.1	0.03241 0.0381 0.003121 0.01064	16.4	14.4
	758.7	541.2 760.0	0.01828 0.0265	11.7	9.71

¹Original data.

continued..

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus was an all glass system which consisted of a manometer, gas handling system, gas buret and solubility bulb equipped with a magnetic stirrer.

The solubility bulb was evacuated and weighed. About $15~{\rm cm}^3$ of solvent was distilled into the bulb, the solvent degassed and the bulb reweighed.

A sample of hydrocarbon was condensed into a calibrated tube; it was vaporized into a known volume and the pressure measured. Equilibrium was established between the gas and the solvent. Pressure was again measured.

SOURCE AND PURITY OF MATERIALS:

- (1) Phillips Petroleum Co. Research grade, 99.88 mole per cent. Removed dissolved air and moisture.
- (2) Commercial absolute alcohol sample fractionated, treated with Mg ethylate, stored in sealed container until used. Dentity, at 25°C 0.78505 g cm⁻³

ESTIMATED ERROR:

 $\delta T/K = \pm 0.005$

 $\delta p/\text{mm Hg} = \pm 0.05$

 $\delta x_1/x_1 = \pm 0.005$ (compilers)

²Calculations for 101.325 kPa (760 mm) were by compilers by extrapolation of data from lower pressures, and by assuming Raoult's law for solvent partial pressure.

COMPO	NENTS:	ORIGINAL MEASUREMENTS:
(1)	2-Methylpropane or isobutane; $C_{\mu}H_{10}$; [75-28-5]	Lebeau, P.
(2)	Water; H ₂ O; [7732-18-5] Ethanol; C ₂ H ₆ O; [64-17-5] Diethylether; C ₄ H ₁₀ O; [60-29-7] Chloroform; CHCl ₃ ; [67-66-3]	Bull. Acad. Roy. Belg. 1908, 300-4.
VARIA	BLES:	PREPARED BY:
	T/K = 290, 291 p/kPa = 102.9 - 104.8	H. L. Clever

EXPERIMENTAL VALUES:

<i>T</i> /K	p/mmHg	Volume	Isobutane/Volume	Solven
290	772		0.13	
1				
290	775		13.2	
lether o	or 1'1'-oxyb	isethane		
291	773		27.9	
form or	trichlorome	thane		
290	786		39.5	
	l 290 lether o 291 form or	1 290 775 lether or 1'1'-oxyb 291 773 form or trichlorome	290 775 lether or 1'1'-oxybisethane 291 773 form or trichloromethane	290 775 13.2 lether or 1'1'-oxybisethane 291 773 27.9 form or trichloromethane

a Not clear whether this is total pressure or isobutane partial pressure. It is probably the total pressure.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Details not given.	 (1) Isobutane. Prepared by the author by the reaction of sodium or calcium in liquid ammonia on isobutyl chloride. The normal boiling point is -10.5 °C and the critical temperature is 134-5 °C. (2) Solvents. No information.
	ESTIMATED ERROR:
	REFERENCES:

Alcohols COMPONENTS: ORIGINAL MEASUREMENTS: (1) 2-Methylpropane; (isobutane); $C_{4}H_{10}$; [75-28-5] Lenoir J-Y.; Renault, P.; Renon, H. (2)1,2-Ethanediol, (Ethylene glycol); J. Chem. Eng. Data, 1971, 16, 340-2 $C_2H_6O_2$; [107-21-1] **VARIABLES:** PREPARED BY: T/K: 298.2 C. L. Young P/kPa: 101.3 EXPERIMENTAL VALUES: Mole fraction at 1 atm* Henry's constant

Calculated by compiler assuming a linear function of $p_{C_4H_{10}}$ vs $x_{C_4H_{10}}$ i.e., $x_{C_uH_{10}}$ (1 atm) = $1/H_{C_uH_{10}}$

 $^{H}C_{4}H_{10}/atm$

320

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

T/K

298.2

A conventional gas-liquid chromatographic unit fitted with a thermal conductivity detector was used. The carrier gas was helium. The value of Henry's law constant was calculated from the retention time. The value applies to very low partial pressures of gas and there may be a substantial difference from that measured at 1 atm. pressure. There is also considerable uncertainty in the value of Henry's constant since surface adsorption was not allowed for although its possible existence was noted.

SOURCE AND PURITY OF MATERIALS:

(1) L'Air Liquide sample; minimum purity 99.9 mole per cent.

 x C₄H₁₀

0.00313

(2) Touzart and Matignon or Serlabo sample; purity 99 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$; $\delta H/atm = \pm 6$ % (estimated by compiler).

COMPONENTS:

- (1) 2-Methylpropane (isobutane); C₄H₁₀; [75-28-5]
- (2) 2-Propanol; C₃H₈O; [67-63-0]

ORIGINAL MEASUREMENTS:

Kretschmer, C.B.; Wiebe, R.

J. Am. Chem. Soc. 1952, 74, 1276-7.

VARIABLES:

T/K = 298.15-323.15P/kPa = 41.46-101.6

PREPARED BY:

H.L. CleverW. Hayduk

EXPERIMENTAL VALUES:

T/K		ssure m Hg Partial ²	Mole Fraction $1,2$	Ostwald Coefficient ² L/cm ³ cm ⁻³	Bunsen Coefficient ² α/cm ³ (STP) cm ⁻³ atm ⁻¹
298.15	355.0	311.0	0.02758		
	525.6	482.4	0.04441		
	753.1	711.0	0.06930		
		760.0	0.0741	24.7	22.8
308.15	761.0	684.0	0.04984		
		760.0	0.0554	18.6	16.6
323.15	762.0	587.8	0.02977		
		760.0	0.0385	13.1	11.1

¹Original data.

Mole fractions at 101.325 kPa were used to determine the following equation for $\ln\,x_1$ and table of smoothed values:

 $\ln x_1 = 2516.7/T - 11.050$ Correlation coefficient = 0.9996

T/K	x	<i>T</i> /K	_ x ₁
298.15	0.0736	313.15	0.0491
303.15	0.0640	323.15	0.0383

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus was an all glass system which consisted of a monometer, gas handling system, gas buret and solubility bulb equipped with a magnetic stirrer.

The solubility bulb was evacuated and weighed. About 15 cm³ of solvent was distilled into the bulb, the solvent degassed and the bulb reweighed.

A sample of hydrocarbon was condensed into a calibrated tube; it was vaporized into a known volume and the pressure measured. Equilibrium was established between the gas and the solvent. Pressure was again measured.

A detailed description of the apparatus and values fo the gas molal volume and 2nd virial coefficient are in (1).

SOURCE AND PURITY OF MATERIALS:

- (1) Phillips Petroleum Co., Research Grade. Specified 99.88 mole percent pure. Treated to remove dissolved gases and moisture.
- (2) Source not given. Fractionated through a 50-plate column, dried with Mg, stored in a sealed container. Density at 25°C 0.78081 g cm⁻³

ESTIMATED ERROR:

 $\delta T/K = 0.005$ $\delta p/mm Hg = 0.05$

 $\delta x_1/x_1 = 0.005$ (compilers)

REFERENCES:

Kretschmer, C.B.; Wiebe, R.
 J. Am. Chem. Soc. 1951, 73, 3778.

²Calculations for 101.325 kPa (760 mm) were by compilers assuming Henry's law, and Raoult's law for solvent partial pressure.

COMPONENTS:

- (1) 2-Methylpropane (isobutane);
 C₄H₁₀; [75-28-5]
- (2) 1-Butanol; C₄H₁₀O; [71-36-3]

ORIGINAL MEASUREMENTS:

Blais, C.; Hayduk, W. J. Chem. Eng. Data <u>1983</u>, 28, 181-184.

VARIABLES:

T/K: 298.15,323.15 P/kPa: 101.325 PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

<i>T</i> /K	Ostwald Coefficient ¹ L/cm ³ cm ⁻³	Bunsen Coefficient ² α/cm ³ (STP)cm ⁻³ atm ⁻¹	Mole Fraction ¹	
298.15	25.3	23.18	0.0889 (0.08890) ³	
323.15	14.1	11.92	0.0486 (0.04860)	

¹Original data.

$$\Delta G^{\circ}/J \text{ mol}^{-1} = -RT \ln x_1 = 615.41 \ T \ln T - 3307.76 \ T$$

$$\ln x_1 = 40.311 - 7.49987 \ln T$$

<i>T/</i> K	10 ⁻⁴ ΔG°/J mol ⁻¹	x	
298.15	5.921	0.08890	
303.15	6.331	0.07848	
313.15	7.165	0.06152	
323.15	8.019	0.04860	

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A volumetric method using a glass apparatus was employed. Degassed solvent contacted the gas while flowing as a thin film, at a constant rate, through an absorption spiral into a solution buret. A constant solvent flow was obtained by means of a calibrated syringe pump. The solution at the end of the spiral was considered saturated. Dry gas was maintained at atmospheric pressure in a gas buret by mechanically raising the mercury level in the buret at an adjustable rate. The solubility was calculated from the constant slope of volume of gas dissolved and volume of solvent injected.

Degassing was accomplished using a two stage vacuum process described by Clever et al. (1).

SOURCE AND PURITY OF MATERIALS:

- 1. Liquid Carbonic. Pure grade of minimum purity 99.0 per cent.
- Canlab (J.T. Baker Company). Spectrophotometric grade of minimum specified purity 99.5 per cent.

ESTIMATED ERROR:

 $\delta T/K = 0.1$ $\delta x_1/x_1 = 0.01$

REFERENCES:

 Clever, H.L.; Battino, R.; Saylor, J.H.; Gross, P.M.
 J. Phys. Chem. <u>1957</u>, 61, 1078.

²Calculated by compiler.

 $^{^3}$ The mole fraction solubility of the original data was used to determine the following equations for ΔG° and $\ln~x_1$ and table of smoothed values:

COMPONENTS:

- (1) 2-Methylpropane (iso-butane); $C_4^{\rm H}{}_{10}$; [75-28-5]
- (2) 2-Ethoxyethanol(ethylcellosolve);
 C₄H₁₀O₂; [110-80-5]

ORIGINAL MEASUREMENTS:

Ezheleva, A.E.; Zorin, A.D. Tr. Khim. Khim. Tech. (Gorkii) 1961, 1, 37-40.

VARIABLES:

T/K: 303.15-343.15

P/kPa: 101.325 and above

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

т/к	Ostwald Coefficient ² L/cm ³ cm ⁻³	Bunsen Coefficient ² α/cm ³ (STP) cm ⁻³ atm ⁻¹	Mole Fraction ¹
303.15	20.6	18.3	0.0780(0.0777) ³
313.15	16.3	14.0	0.0625(0.0628)
323.15	13.7	11.3	0.0527(0.0514)
333.15	10.3	8.28	0.0404(0.0426)
343.15	9.27	7.21	0.0368(0.0357)

¹Original data given as the inverse of Henry's constant which is equivalent to mole fraction at a gas partial pressure of 101.325 kPa.

$$\ln x_1 = 2020.3/T - 9.2195$$

Correlation coefficient = 0.9942

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of a two-chamber, rocking device with separate gas and liquid chambers joined by two tubes and microvalves. The gas chamber was equipped with a pressure gauge. After evacuation, gas and deaerated solvent were separately charged, and then contacted by opening the microvalves and by rocking. The solubility was calculated from a knowledge of the volume of the solvent charged, and the initial and final gas pressures.

The solvent was considered non-volatile and the gas pressure was considered to be the total pressure.

SOURCE AND PURITY OF MATERIALS:

- Source and purity not given. Gas purified by low temperature fractionation and analyzed by gas chromatography.
- Source and purity not given. Refractive index measured:

$$n_D^{20} = 1.4078$$

ESTIMATED ERROR:

 $\delta T/K = 0.05$

 $\delta x_1/x_1 = 0.05$

(estimated by compiler)

²Ostwald and Bunsen coefficients calculated by compiler using authors' assumption that solvent is non-volatile.

³From equation of smoothed data:

ORIGINAL MEASUREMENTS: COMPONENTS: (1) 2-Methylpropane; (isobutane) Lenoir, J-Y.; Renault, P.; Renon, H. $C_{\mu}H_{10}$; [75-28-5] (2) Phenol; C_6H_6O ; [108-95-2] J. Chem. Eng. Data, 1971, 16, 340-2 **VARIABLES:** PREPARED BY: T/K: 323.2 C. L. Young 101.3 P/kPa: EXPERIMENTAL VALUES:

T/K	Henry's constant HC4H10	Mole fraction at 1 atm* **C4H10
323.2	67.0	0.0149

* Calculated by compiler assuming a linear function of $p_{C_4H_{10}}$ vs $x_{C_4H_{10}}$, i.e., $x_{C_4H_{10}}$ (1 atm) = $1/H_{C_4H_{10}}$

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

A conventional gas-liquid chromatographic unit fitted with a thermal conductivity detector was used. The carrier gas was helium. The value of Henry's law constant was calculated from the retention time. The value applies to very low partial pressures of gas and there may be a substantial difference from that measured at 1 atm. pressure. There is also considerable uncertainty in the value of Henry's constant since surface adsorption was not allowed for although its possible existence was noted.

SOURCE AND PURITY OF MATERIALS:

- (1) L'Air Liquide sample; minimum purity 99.9 mole per cent.
- (2) Touzart and Matignon or Serlabo sample; purity 99 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$; $\delta H/atm = \pm 6\%$ (estimated by compiler).

COMPONENTS:

- 1. Propane, 2-methyl-, (isobutane) C_4H_{10} ; [75-28-5]
- 2. Propanol, oxybis-, (Dipropylene glycol); $C_6H_{14}O_3$; [25265-71-8]

ORIGINAL MEASUREMENTS:

Lenoir, J-Y.; Renault, P.; Renon, H.

J. Chem. Eng. Data 1971, 16, 340-2

VARIABLES:

T/K: 298.2-343.2

P/kPa: 101.3

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

T/K	Henry's constant HC4H10	Mole fraction at 1 atm* **C4H10
298.2	42.4	0.0236
323.2	53.7	0.0186
343.2	74.3	0.0135

* Calculated by compiler assuming a linear function of $p_{C_4H_{10}}$ vs $x_{C_4H_{10}}$, i.e., $x_{C_4H_{10}}$ (1 atm) = $1/H_{C_4H_{10}}$

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

A conventional gas-liquid chromatographic unit fitted with a thermal conductivity detector was used. The carrier gas was helium. The value of Henry's law constant was calculated from the retention time. The value applies to very low partial pressures of gas and there may be a substantial difference from that measured at l atm. pressure. There is also considerable uncertainty in the value of Henry's constant since surface adsorption was not allowed for although its possible existence was noted.

SOURCE AND PURITY OF MATERIALS:

- (1) L'Air Liquide sample, minimum purity 99.9 mole per cent.
- (2) Touzart and Matignon or Serlabo sample, purity 99 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$; $\delta H/atm = \pm 6\%$ (estimated by compiler).

ORIGINAL MEASUREMENTS: COMPONENTS: (1) 2-Methylpropane, (isobutane); Gerrard, W. C_4H_{10} ; [75-28-5] Solubility of Gases and Liquids, Plenum, New York, 1976, Chapter 12. (2) Benzyl alcohol, (Benzenemethanol) C_7H_0O ; [100-51-6] VARIABLES: PREPARED BY: T/K: 273.15 P/kPa: 13.3-101.3 C.L. Young

				
EXPERIMENTAL VALUES:				
T/K	P/mmHg	P/kPa	Mole fraction of 2-methyl propane in liquid, $x_{C_4H_{10}}$	
273.15	100	13.3	0.012	
	200	26.7	0.020	
	300	40.0	0.028	
	400	53.3	0.037	
	500	66.7	0.049	
	600	80.0	0.064	
	700	93.3	0.086	
	760	101.3	0.107	

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Gas was passed into a known weight of pure liquid in a bubbler tube at a total pressure measured by a manometer assembly. The amount of absorbed gas was estimated by weighing. The temperature was manually controlled to within 0.2K. The apparatus and procedure are described by Gerrard (1,2).

SOURCE AND PURITY OF MATERIALS:

No details given.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \ \delta x/x = \pm 3\%$ (estimated by compiler).

- REFERENCES: 1. Gerrard, W. J. Appl. Chem. Biotechnol. 1972 22, 623-650.
- Gerrard, W. Solubility of Gases and Liquids, Plenum Press. New York, 1976 Chapter 1.

EXPERIMENTAL VALUES:

			•
т/к	P/mmHg	P/kPa	Mole fraction of 2-methyl propane in liquid, $x_{C_4H_{10}}$
273.15	100	13.3	0.045
	200	26.7	0.088
	300	40.0	0.132
	400	53.3	0.178
	500	66.7	0.224
	600	80.0	0.282
	700	93.3	0.344
	760	101.3	0.386

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

Gas was passed into a known weight of pure liquid in a bubbler tube at a total pressure measured by a manometer assembly. The amount of absorbed gas was estimated by weighing. The temperature was manually controlled to within 0.2K. The apparatus and procedure are described by Gerrard (1,2).

SOURCE AND PURITY OF MATERIALS;

No details given.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$; $\delta x/x = \pm 3\%$ (estimated by compiler)

- Gerrard, W.
 J. Appl. Chem. Biotechnol. <u>1972</u>
 22, 623-650.
- Gerrard, W. Solubility of Gases and Liquids, Plenum Press, New York, 1976, Chapter 1.