MODELS OF GAS-LIQUID SOLUBILITIES

Volume II

A thesis submitted
by

ANNE-LISE BUHL JENSEN,

M. Sc. , Denmark (Chemical Engineering)

A candidate for the degree of

Doctor of Philosophy

Department of Chemical Engineering &

Applied Chemistry

THE UNIVERSITY OF ASTON IN BIRMINGHAM

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Appendix 1 - The AGAPE equations for the multicomponent case

The AGAPE equations for the binary mixture were derived in section 2.11. The similar equations for the multicomponent case are as follows :

The excess Gibbs free energy :

$$\frac{g^E}{RT} = \sum_{i=1}^{N} x_i \ln \frac{\lambda_i^A}{x_i} + \frac{z}{2} \sum_{i=1}^{N} x_i\, q_i \ln \frac{\theta_i^A}{\lambda_i^A} - \frac{z}{2} \sum_{i=1}^{N} \left[x_i\, C_i^A \ln \left(\sum_{j=1}^{N} \lambda_j^A\, \tau_{ij}^A \right) \right] \qquad \text{(A1.1)}$$

The activity coefficient for component i :

$$\ln \gamma_i = \ln \frac{\lambda_i^A}{x_i} + \sum_{j=1}^{N} \frac{\lambda_j^A}{\tau_{ij}} (r_j - r_i) + \frac{z}{2} q_i \left[\ln \frac{\theta_i^A}{\lambda_i^A} - 1 \right] - \frac{z}{2} \left(C_i^A \ln \left(\sum_{j=1}^{N} \lambda_i^A\, \tau_{ji}^A \right) + \sum_{j=1}^{N} C_j^A\, \lambda_k^A \frac{r_i}{r_j} \left[\frac{\tau_{ij}^A}{\sum_{k=1}^{N} \lambda_k^A \tau_{kj}^A} - 1 \right] \right) \qquad \text{(A1.2)}$$

where

$$C_i^A = \prod_{j=1\, j \neq i}^{N} \frac{\left(\Phi_{ji} \frac{r_i}{r_j} - \Phi_{ii} \right)}{(\Phi_{ji} - \Phi_{ii})} \quad ; \quad \tau_{ji}^A = \exp \left[- \frac{L}{RT} (\Phi_{ji} - \Phi_{ii}) \right]$$

$$\lambda_i^A = \frac{x_i\, r_i}{\sum_{i=1}^{N} x_i\, r_i} \quad ; \quad \theta_i^A = \frac{x_i\, q_i}{\sum_{i=1}^{N} x_i\, q_i} \qquad \text{(A1.3)}$$

and

$$r_i = \frac{V_i^m}{V_1^m}$$

$$q_i = \frac{A_{Wi}}{A_{W1}}$$

Again, the parameters r_i are defined as the ratio of a characteristic volume (molar volume or van der Waals volume or another suitable volume) and is in this case chosen to define the characteristic unit size of the lattice and hence, $r_1 = 1.0$. The parameters q_i is the ratio of van der Waals surface area and again, $q_1 = 1.0$.

Compared to the similar equations in Table 2-4 the AGAPE equations look similar to the UNIQUAC equations, especially in complexity. There is, though, one very important difference, the AGAPE equations use only molecular and volume parameters for the pure compounds, whereas UNIQUAC includes binary parameters.

Appendix 2 - Prediction results using the AGAPE and the AGAPE-FIT methods

The tables in this section (Table A2-1 to A2-10) show phase equilibrium data, both experimental data and results obtained using the AGAPE equations as described in section 2.11. The first row shows the components in the binary mixture, the experimental temperature and the AGAPE method applied either the GLP method (described in section 2.11.10) or the AGAPE-FIT method (described in section 2.11.14) using the relevant computer programs. The three columns display the experimental values of the liquid phase mole fraction of component 1, the experimental vapour phase mole fraction of component 1, and the experimental total pressure. The next two columns show the predicted results obtained by employing the AGAPE equations to the experimental liquid mole fractions. The predicted values of the vapour mole fraction is first, then follows the predicted total pressure. All data are from Kakhu et al. (1995).

Ar+O_2	84 K	Fit		
x_1	y_1-exp	P-exp (10^5 Pa)	y_1-pred	P-pred (10^5 Pa)
0	0	0.9489	0	0.9489
0.1	0.1482	1.0045	0.1489	1.0054
0.2	0.2738	1.0535	0.2746	1.0547
0.3	0.3838	1.0967	0.3842	1.0979
0.4	0.4826	1.1347	0.4827	1.1357
0.5	0.574	1.1682	0.5737	1.1689
0.6	0.6606	1.1975	0.66	1.198
0.7	0.7446	1.223	0.744	1.2234
0.8	0.828	1.2449	0.8275	1.2452
0.9	0.9126	1.2634	0.9123	1.2637
1	1	1.2786	1	1.2786

Table A2-1. Argon (1) and oxygen (2) at 84 K. Vapour mole fractions and total pressures predicted by the AGAPE-FIT method and experimental values.

N_2+CO	83.82 K	GLP		
x_1	y_1-pred	P-pred (10^5 Pa)	y_1-exp	P-exp (10^5 Pa)
1	1		1	
0.8937	0.8383	1.3606	0.8267	1.3812
0.8054	0.7193	1.4299	0.7058	1.4627
0.686	0.5765	1.5221	0.5664	1.5648
0.5588	0.4426	1.6187	0.439	1.665
0.4933	0.3798	1.6679	0.3796	1.7136
0.3878	0.2859	1.7464	0.2905	1.7881
0.2865	0.2032	1.8212	0.2106	1.8558
0.1328	0.0892	1.9337	0.0959	1.9522
0	0		0	

Table A2-2. Nitrogen (1) and carbon monoxide (2) at 83.82 K. Vapour mole fractions and total pressures predicted by the AGAPE method and experimental values.

CS_2+C_3H_6O	298 K	Fit		
x_1	y_1-exp	P-exp (10^5 Pa)	y_1-pred	P-pred (10^5 Pa)
0.074	0.286	0.4292	0.3098	0.4164
0.114	0.39	0.4745	0.393	0.4578
0.214	0.5	0.5385	0.5087	0.5254
0.336	0.584	0.5732	0.5744	0.5649
0.425	0.616	0.5865	0.6012	0.5782
0.648	0.675	0.5999	0.6485	0.5886
0.766	0.71	0.5999	0.6874	0.5839
0.828	0.736	0.5919	0.7223	0.5747
0.915	0.806	0.5639	0.8094	0.5444

Table A2-3. Carbon disulfide (1) and acetone (2) at 298 K. Vapour mole fractions and total pressures predicted by the AGAPE-FIT method and experimental values.

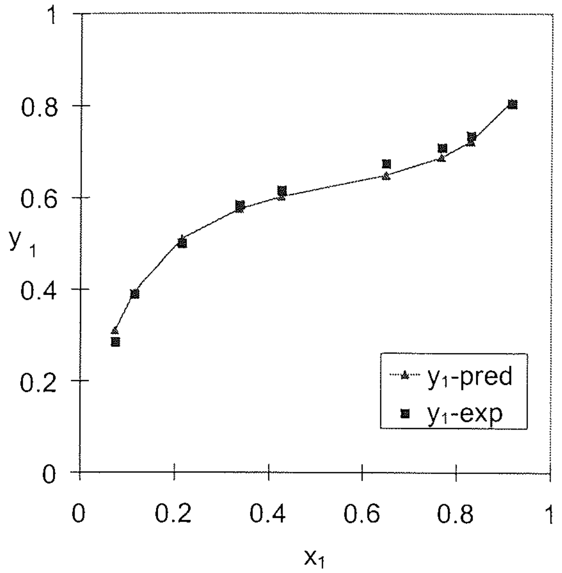

Figure A2.1. Carbon disulfide (1) and acetone (2) at 298 K. Vapour mole fractions predicted by the AGAPE-FIT method (line and ▲) and experimental values (■).

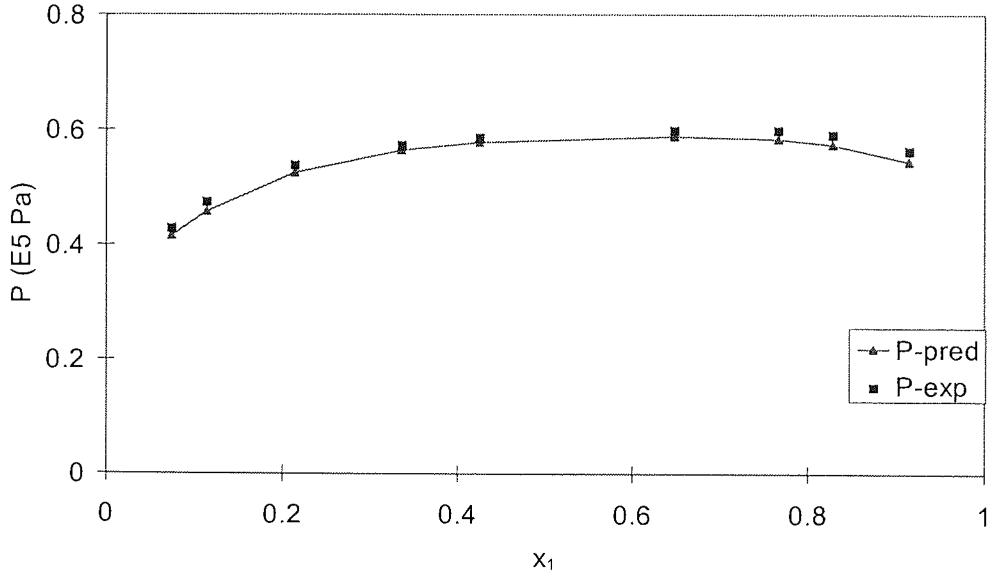

Figure A2.2. Carbon disulfide (1) and acetone (2) at 298 K. Total pressure predicted by the AGAPE-FIT method (line and ▲) and experimental values (■).

$CHCl_3+C_2H_5OH$		328 K	Fit	
x_1	y_1-exp	P-exp (10^5 Pa)	y_1-pred	P-pred (10^5 Pa)
1	1	0.824	1	0.8241
0.9	0.877	0.868	0.885	0.8521
0.8	0.826	0.869	0.8234	0.8526
0.7	0.791	0.858	0.7827	0.8417
0.6	0.76	0.838	0.749	0.8237
0.5	0.725	0.807	0.7135	0.797
0.4	0.677	0.761	0.6687	0.7574
0.3	0.611	0.695	0.6049	0.6991
0.2	0.499	0.603	0.5054	0.6169
0.1	0.305	0.486	0.3348	0.508
0	0	0.373	0	0.3741

Table A2-4. Chloroform (1) and ethanol (2) at 328 K. Vapour mole fractions and total pressures predicted by the AGAPE-FIT method and experimental values.

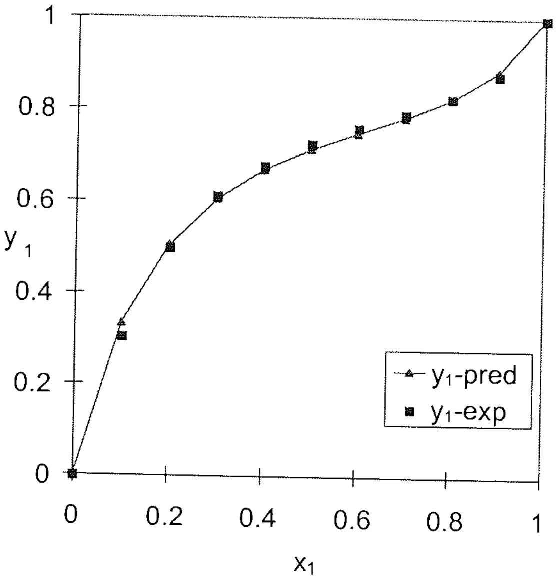

Figure A2.3. Chloroform (1) and ethanol (2) at 328 K. Vapour mole fractions predicted by the AGAPE-FIT method and (line and ▲) and experimental values (■).

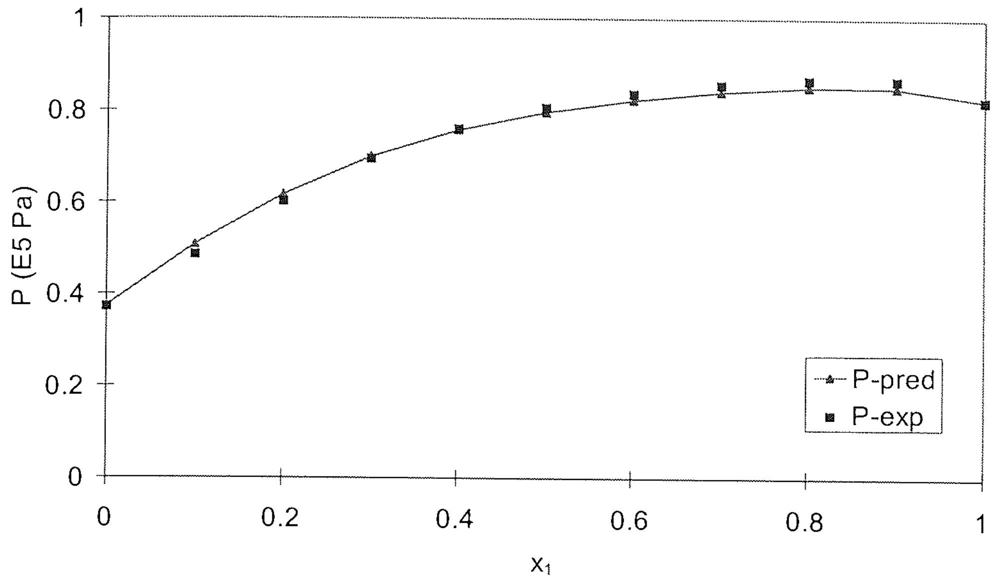

Figure A2.4. Chloroform (1) and ethanol (2) at 328 K. Total pressure predicted by the AGAPE-FIT method (line and ▲) and experimental values (■).

$Xe+CF_4$	159.01 K	Fit		
x_1	y_1-exp	P-exp (10^5 Pa)	y_1-pred	P-pred (10^5 Pa)
0	0	2.445	0	2.4765
0.0743	0.10944	2.571	0.108	2.5977
0.2476	0.21007	2.614	0.2019	2.6308
0.363	0.23971	2.578	0.2176	2.6103
0.4339	0.25099	2.56	0.2203	2.6031
0.5801	0.26314	2.517	0.2223	2.5943
0.7258	0.27482	2.459	0.2368	2.5013
0.7788	0.28062	2.42	0.252	2.3983
0.8876	0.3116	2.221	0.3349	1.9219
1	1	0.714	1	0.709

Table A2-5. Xenon (1) and carbon tetrafluoride (2) at 159.01 K. Vapour mole fractions and total pressures predicted by the AGAPE-FIT method and experimental values.

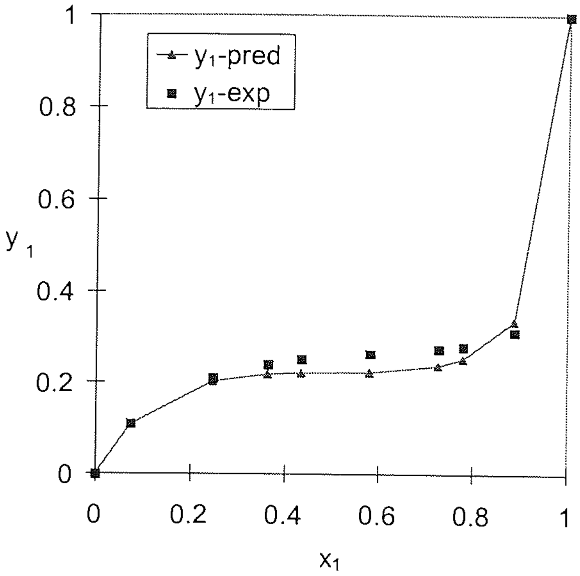

Figure A2.5. Xenon (1) and carbon tetrafluoride (2) at 159.01 K. Vapour mole fractions predicted by the AGAPE-FIT method line and ▲) and experimental values (■).

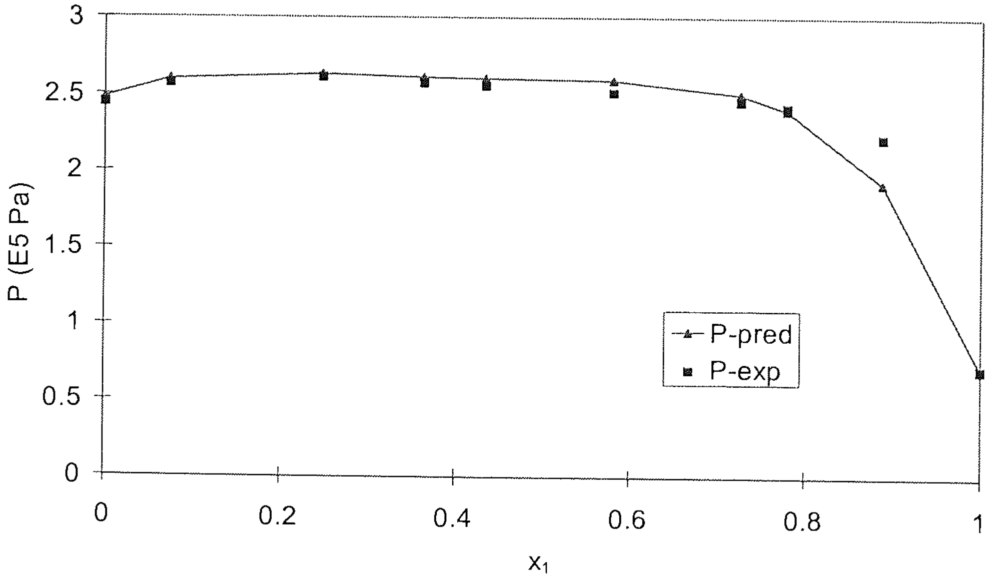

Figure A2.6. Xenon (1) and carbon tetrafluoride (2) at 159.01 K. Total pressure predicted by the AGAPE-FIT method (line and ▲) and experimental values (■).

Appendix 3 - Solubility of various solutes dissolved in various solvents

Solubility data for various solutes dissolved in various solvents at T=298.15 K and p_{solute} = 101.325 kPa. All the data shown are liquid mole fraction for the solute * 10000 and they are from Fogg and Gerrard (1991) or IUPAC Solubility Data Series (Clever, 1979 (vol. 1), Clever, 1980 (vol. 4), Young, 1981 (vol. 5/6), Battino, 1981 (vol. 7), Hayduk, 1982 (vol. 9), Battino, 1982 (vol. 10), Hayduk, 1986 (vol. 24), and Clever and Young, 1987 (vol. 27/28)).

solvent	**formula**	**solute - H_2 Solubility *10000 ref. Sol. Data.Ser, vol 5/6.**	**solute - N_2 Solubility *10000 ref. Sol. Data Ser. vol 10**	**solute - He Solubility *10000 ref. Sol. Data Ser. vol. 1**	**solute - CO Solubility *10000 ref. Fogg and Gerrard (1991)**
n-hexane	n- C_6H_{14}	6.63	13.9	2.57	17.375
diethyl ether	$C_2H_5OC_2H_5$	6.24			
cyclo-hexane	c- C_6H_{12}	4.14	7.68	1.22	9.99
carbon tetrachloride	CCl_4	3.225	6.41		8.65
m- xylene	1,3-C_8H_{10}	4.15	6.12	1.03, 1.06, 1.12	
methyl acetate	$C_3H_6O_2$	3.0	5.97		8.50
acetone	C_3H_6O	3.01	5.421	1.09	7.80
benzene	C_6H_6	2.591	4.45	0.759	6.50
chloroform	CCl_3H	2.2	4.45		6.65
chlorobenzene	C_6H_5Cl	2.56	4.27	0.696	6.31
nitrobenzene	$C_6H_5NO_2$	1.56	2.6, 2.64	0.377	3.85
methanol	CH_3OH	1.61	2.76	0.594	3.27
carbon disulfide	CS_2	1.593	2.215	0.39	3.60
aniline	$C_6H_5NH_2$	1.07	1.15		1.97
water	H_2O	0.1411	0.1183	0.06997	0.172
ethanol	C_2H_5OH	2.06	3.57	0.791	4.49
1-propanol	C_3H_7OH	2.31	4.02		5.193
1,2-dichloro ethane	1,2- $C_2H_4Cl_2$	1.77			
ideal solubility		8 (Ref. Hildebrand and Scott, 1964)	10 (Ref. Hildebrand and Scott, 1964)		12.8 (Ref. Hildebrand and Scott, 1964)

Table A3-1. Solubilities of selected solutes dissolved in various solvents (continued over).

Solvent	**solute - O_2 Solubility *10000 Ref. Sol. Data Ser. vol. 17**	**solute - CH_4 Solubility *10000 Ref. Sol. Data Ser., vol. 27/28 and Fogg and Gerrard, 1991**	**solute - C_2H_4 Solubility *10000 Ref. Fogg and Gerrard, 1991.**	**solute - Ar Solubility *10000 Ref. Sol. Data Ser. vol. 4**	**solute - C_2H_2 Solubility *10000 Ref. Fogg and Gerrard, 1991.**
n-hexane	19.8	50.8	193.0	25.2	470
diethyl ether					
cyclo-hexane	12.3	32.7		11.4	
carbon tetrachloride	12.0	28.56	148	13.5	117
m- xylene	11.96	27.13		11.88	
methyl acetate	8.905		116		684
acetone	8.44	18.5	111	9.03	644
benzene	8.10	20.9	118.5	8.82	177
chloroform				5.92 (T=295.15 K)	140
chlorobenzene	7.888	19.86	121	8.52	148
nitrobenzene	4.95	10.6	79	4.39	
methanol	4.15	8.71	47(T=293.2 K)	4.47	190
carbon disulfide	4.39	13.09		4.863	
aniline	2.26		48		
water	0.2293	0.2548	0.8582	0.2519	7.40
ethanol	5.825	12.8		6.257	466
1-propanol	5.03	15.6		7.77	
1,2-dichloro ethane			89		214
dichloromethane					
ideal solubility	13.2 (Ref. Hildebrand and Scott, 1964)	35	148.2	16 (Ref. Hildebrand and Scott, 1964)	206.7

Table A3-1. Solubilities of selected solutes dissolved in various solvents (continued over).

Solvent	**solute - C_2H_6 Solubility *10000 Ref. Fogg and Gerrard, 1991.**	**solute - Ne Solubility *10000 Ref. Sol. Data Ser., vol. 10**	**solute - n-C_3H_8 Solubility *10000 Ref. Fogg and Gerrard (1991)**	**solute - CO_2 Solubility * 10000 Ref. Fogg and Gerrard (1991)**	**solute - n-C_4H_{10} Solubility * 10000 Ref. Fogg and Gerrard (1991)**
n-hexane	317	3.80	1160	121.09	3860
diethyl ether					
cyclo-hexane	233	1.845	910	75.9	
carbon tetrachloride	211		813	106	3390
m- xylene		1.615	731	107	3530
methyl acetate	105			217	
acetone	97.2			199	
benzene	149	1.151	573	91.2	
chloroform				128	
chlorobenzene	146	0.986	570	96.0	2690
nitrobenzene	73.5	0.509	247	101.5	711
methanol	39.3	0.804	115	63.9	398
carbon disulfide	107	0.59	446	32.8	
aniline					
water	0.340	0.08152	0.2732	6.116	0.2244
ethanol	66.6	1.090	228	68.9	815
1-propanol				77.2	
1,2-dichloro ethane				113	
dichloromethane					
ideal solubility	246.2			167	

Table A3-1. Solubilities of selected solutes dissolved in various solvents.

The collected solubility data are illustrated in Figures A3-1 to A3-16. For the majority of the charts, the solubility * 10000 is along the y-axis and the various solvents are along the x-axis whereas the different columns represent the solutes.

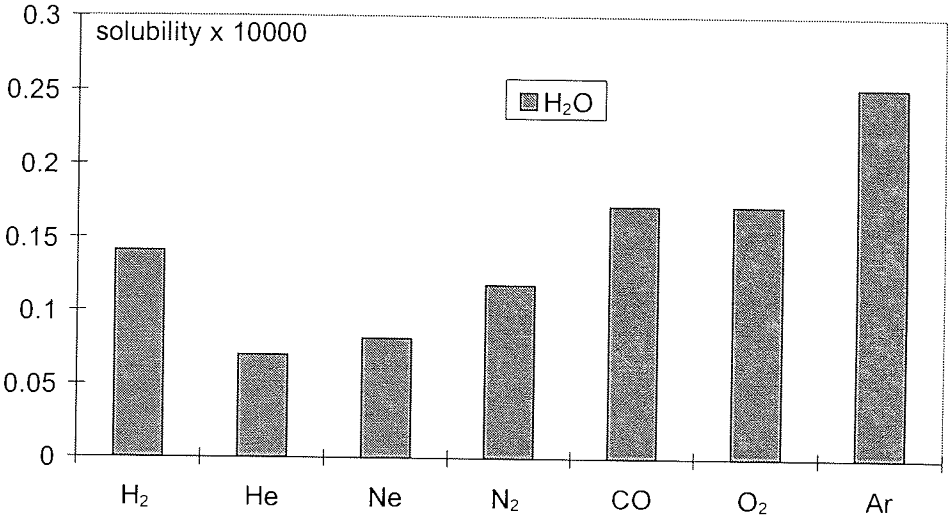

Figure A3.1. Solubility of various solutes dissolved in the solvent WATER.

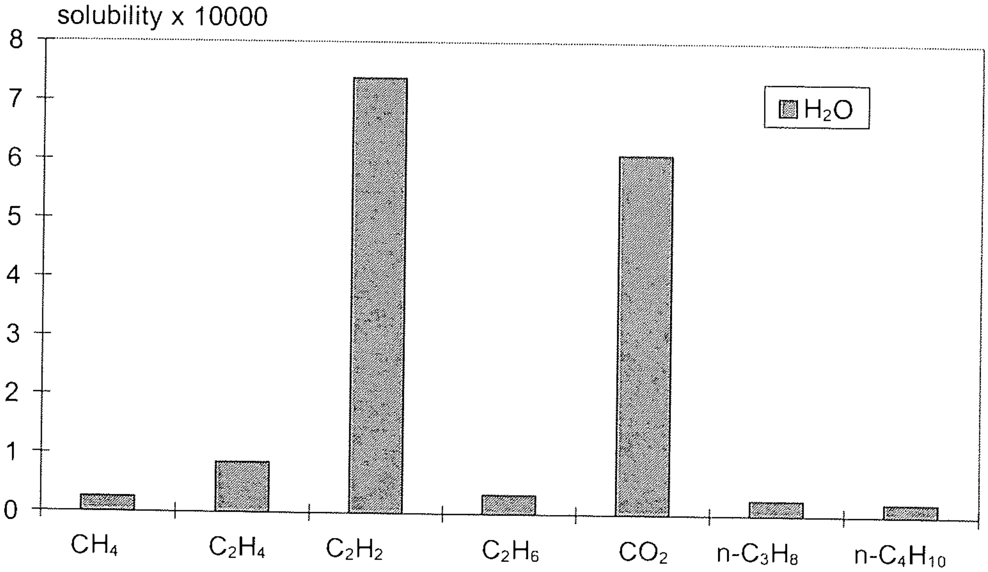

Figure A3.2. Solubility of various solutes dissolved in the solvent WATER.

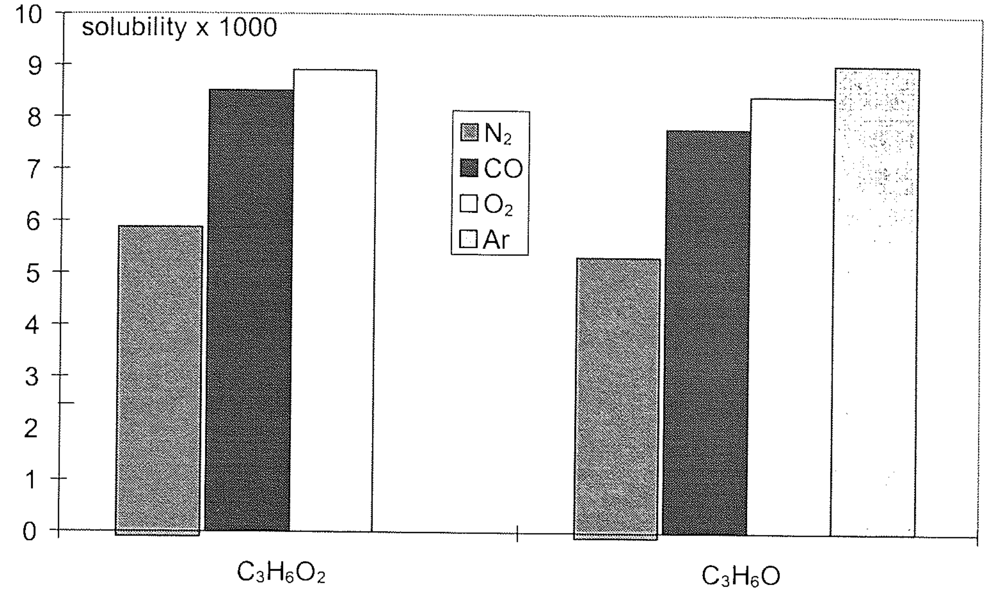

Figure A3.3. Solubilities of various solutes dissolved in methyl acetate ($C_3H_6O_2$) and acetone (C_3H_6O).

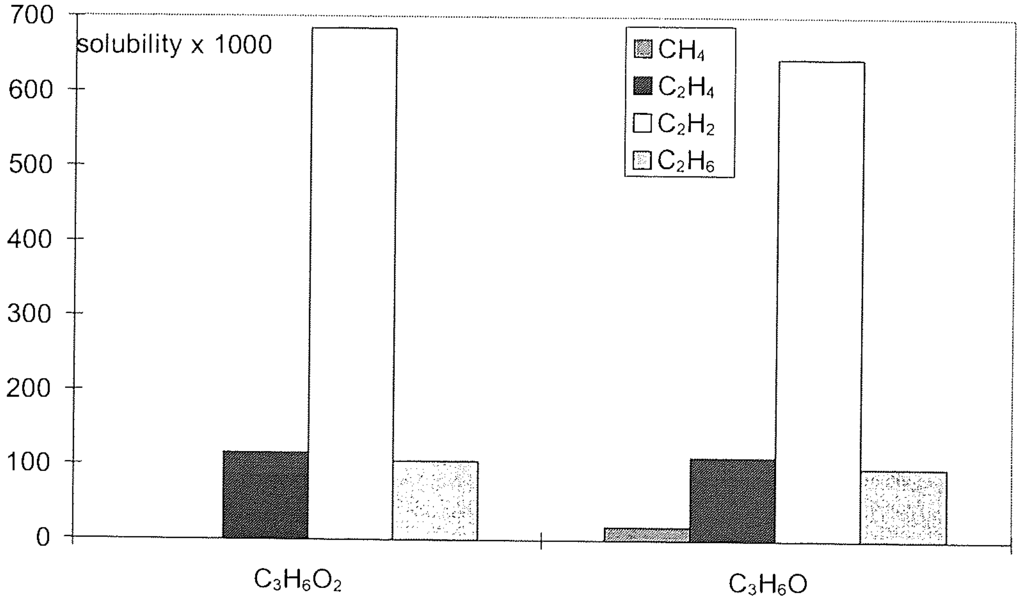

Figure A3.4. Solubilities of various solutes dissolved in methyl acetate ($C_3H_6O_2$) and acetone (C_3H_6O).

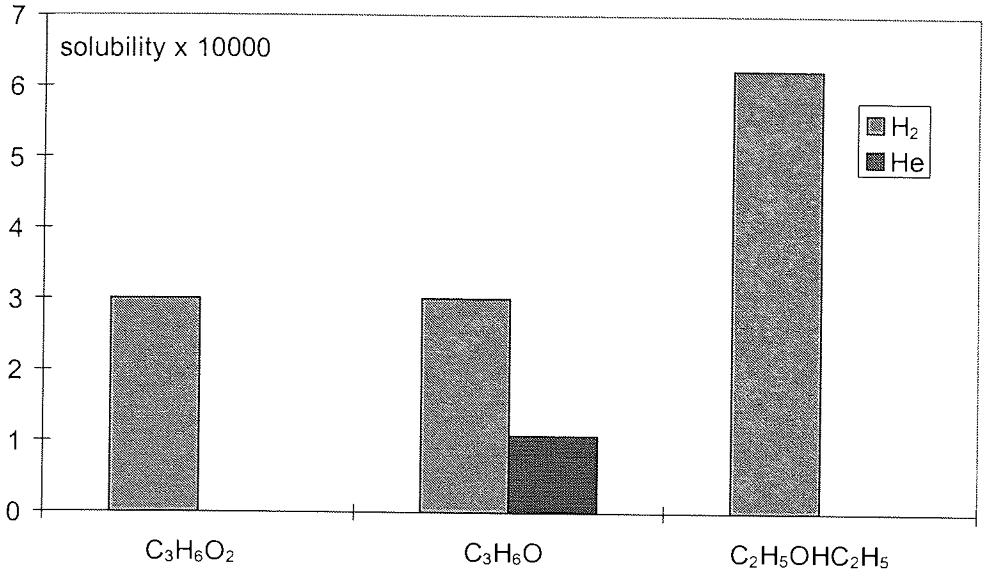

Figure A3.5. Solubilities of various solutes dissolved in methyl acetate ($C_3H_6O_2$), acetone (C_3H_6O), and diethyl ether.

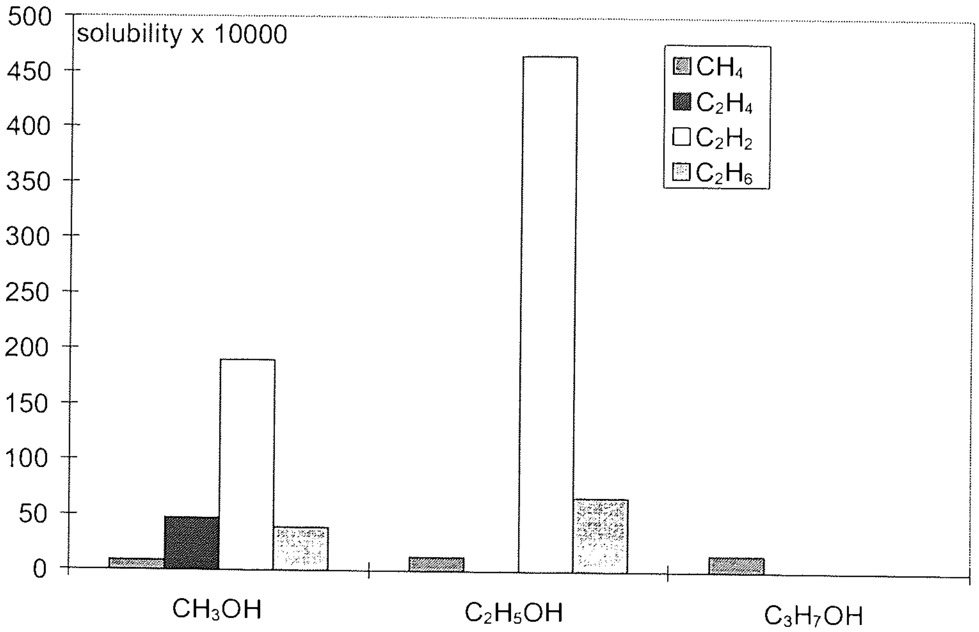

Figure A3.6. Solubilities of various solutes dissolved in methanol, ethanol, and 1-propanol.

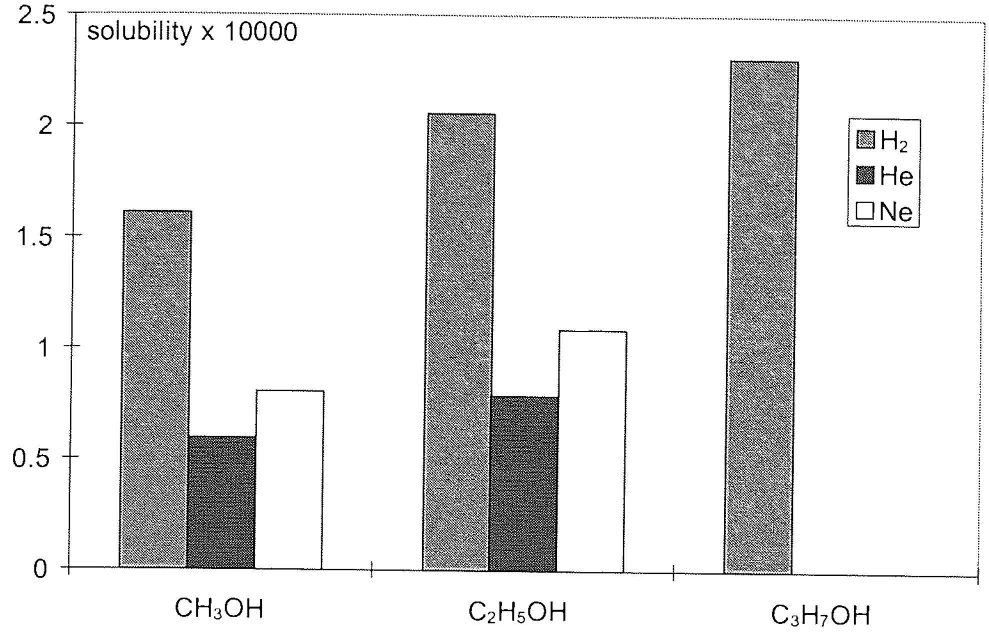

Figure A3.7. Solubilities of various solutes dissolved in methanol, ethanol, and 1-propanol.

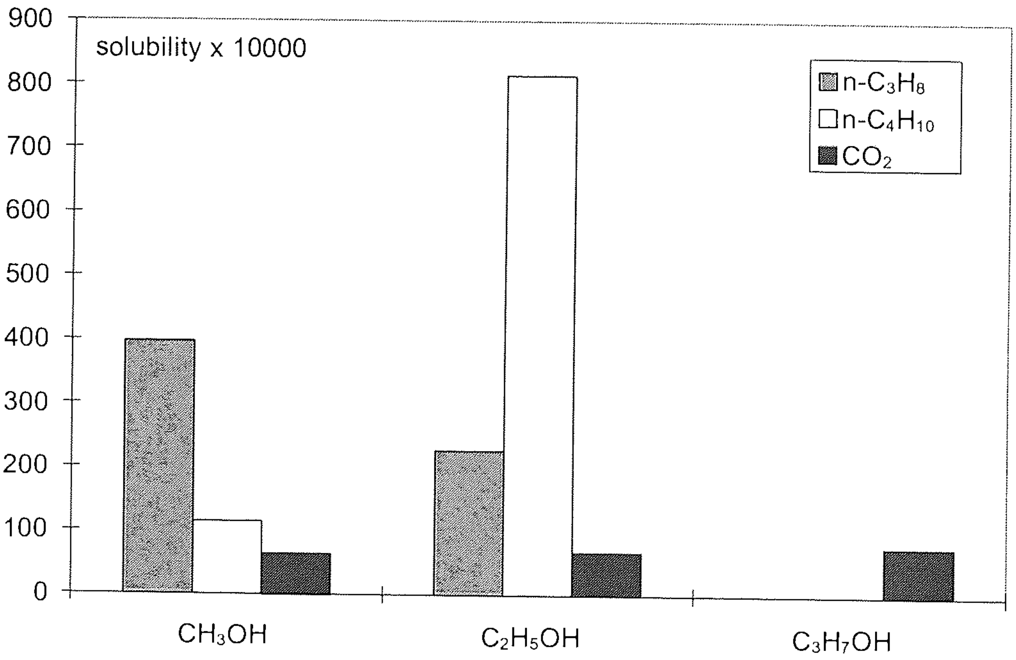

Figure A3.8. Solubilities of various solutes dissolved in methanol, ethanol, and 1-propanol.

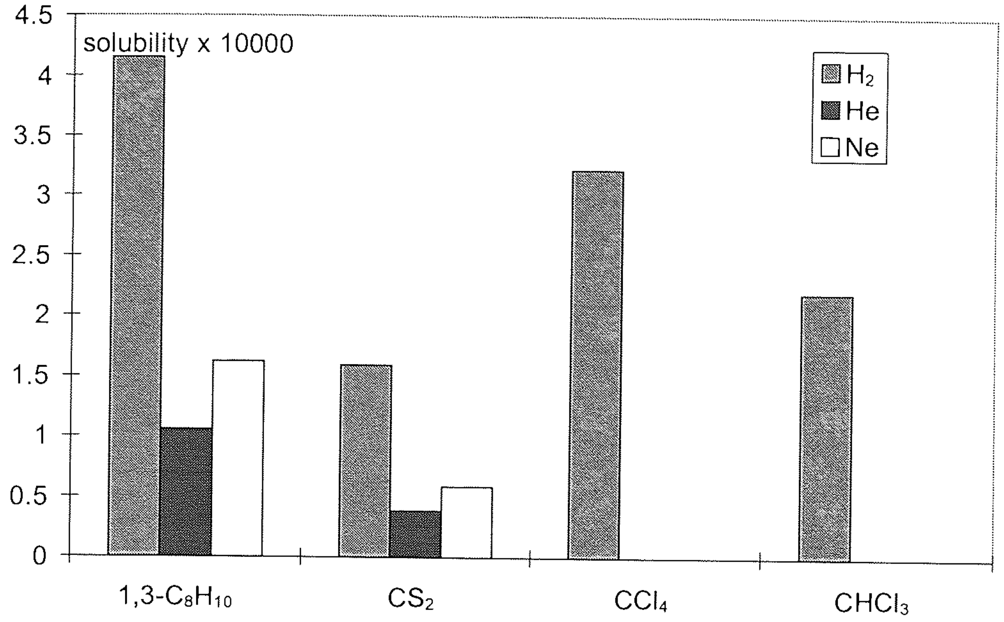

Figure A3.9. Solubilities of various solutes dissolved in m-xylene, carbon disulfide, carbon tetrachloride, and chloroform.

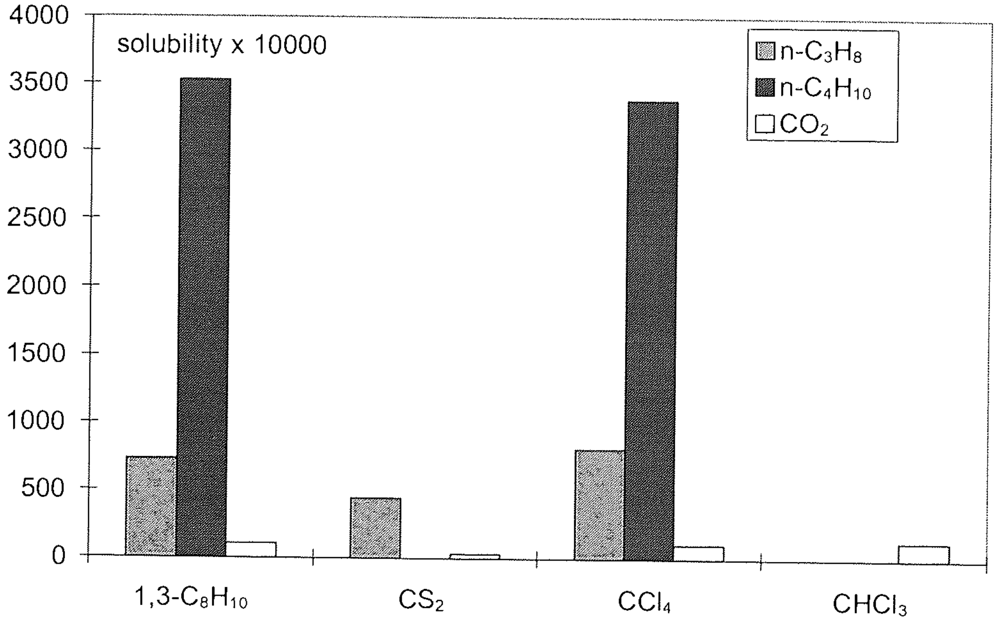

Figure A3.10. Solubilities of various solutes dissolved in m-xylene, carbon disulfide, carbon tetrachloride, and chloroform.

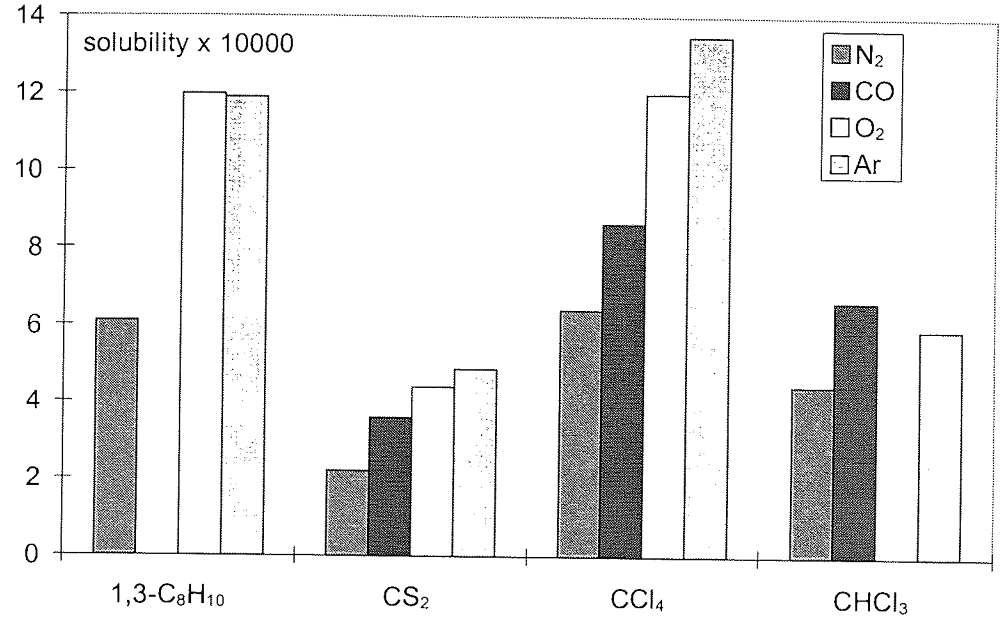

Figure A3.11. Solubilities of various solutes dissolved in m-xylene, carbon disulfide, carbon tetrachloride, and chloroform.

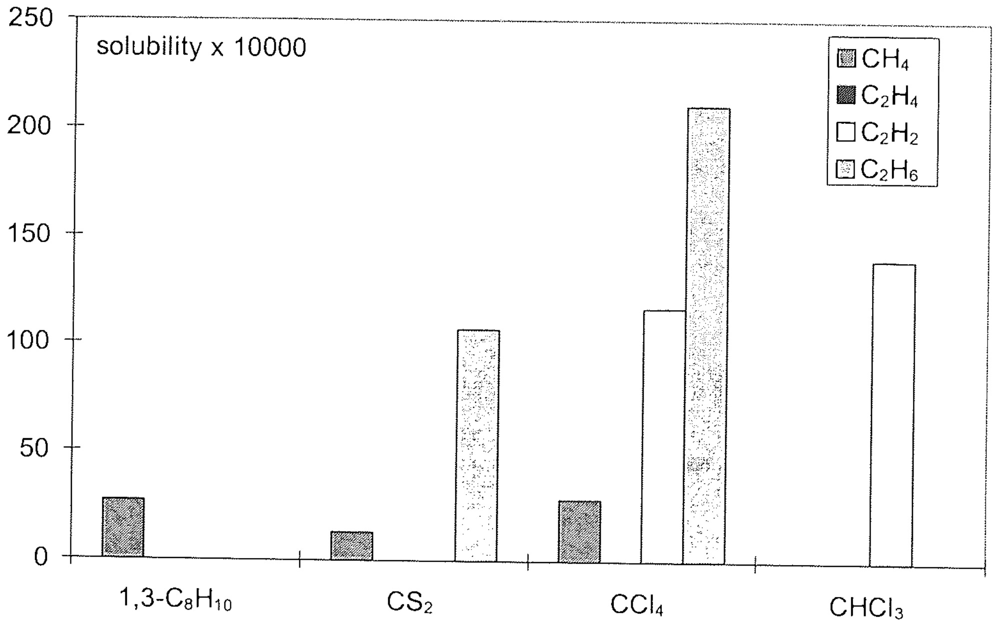

Figure A3.12. Solubilities of various solutes dissolved in m-xylene, carbon disulfide, carbon tetrachloride, and chloroform.

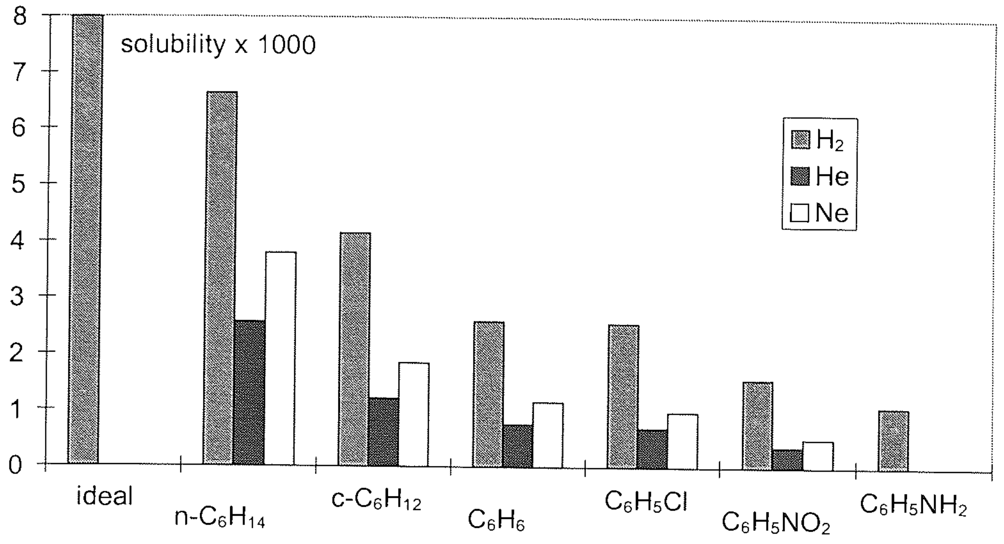

Figure A3.13. Solubilities of various solutes dissolved in various solvents.

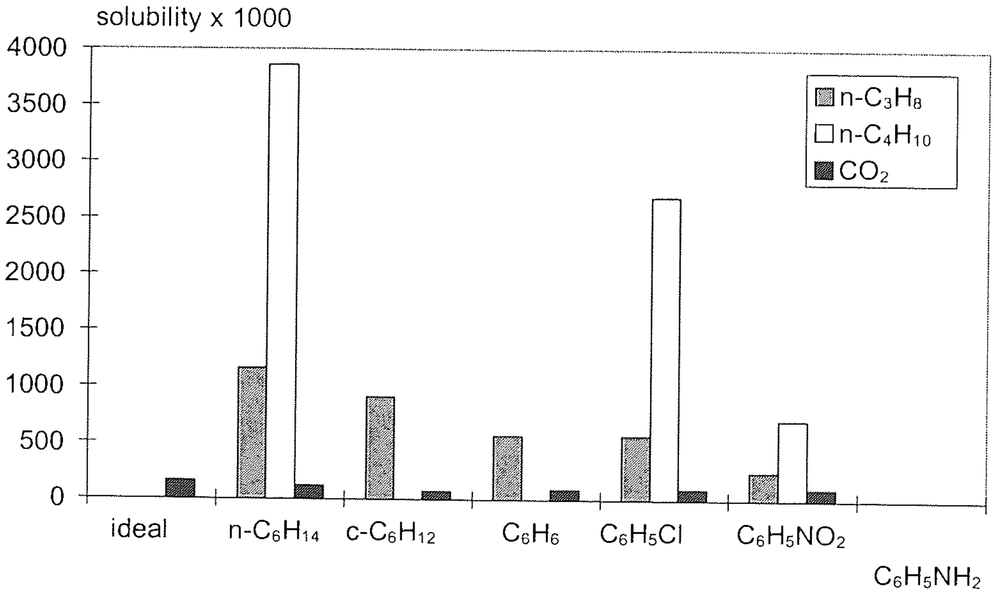

Figure A3.14. Solubilities of various solutes dissolved in various solvents.

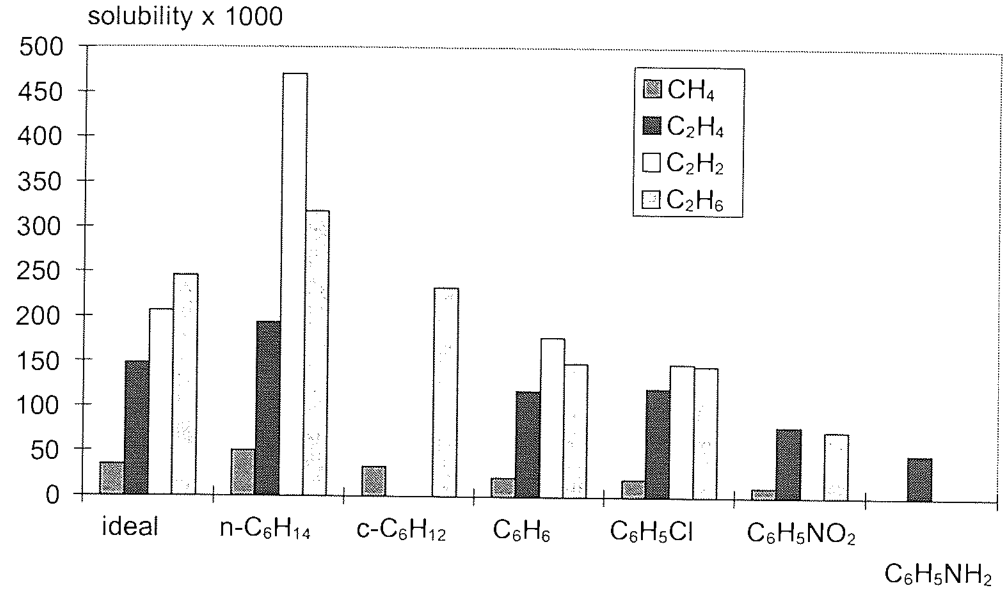

Figure A3.15. Solubilities of various solutes dissolved in various solvents

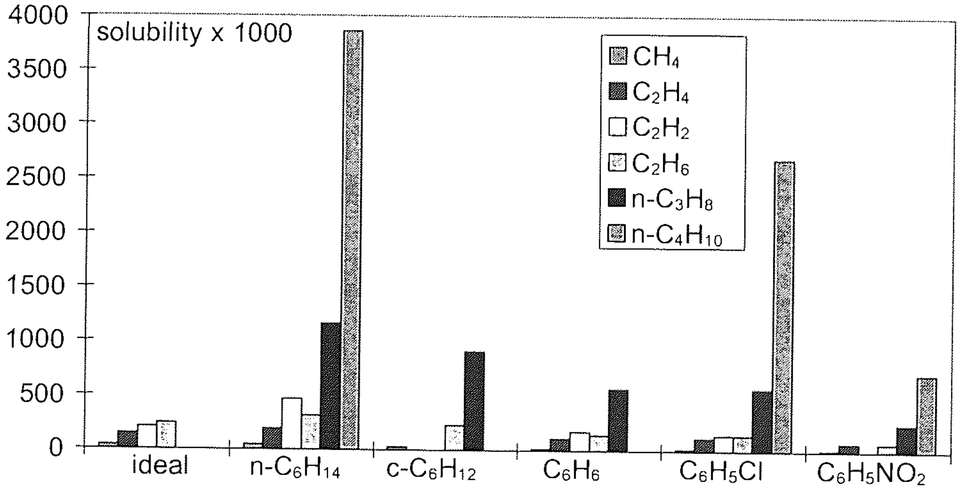

Figure A3.16. Solubilities of various solutes dissolved in various solvents.

Figure A3.16 is a combination of Figures A3.14 and A3.15.

Appendix 4 - Results of Mohammadi's (1986) calculations

Table A4-1 shows the results obtained by Mohammadi (1986) by employing equation (4.2) for the mentioned mixtures. The liquid mole fractions of the solute (the solubilities) are all experimental values at 298.15 K and at a pressure of the solute of 101.325 kPa.

mixture solvent-solute	PE(uv) (equation (4.2)) Mohammadi (1986)	x_{solute} Mohammadi (1986)	ln x_{solute} Mohammadi (1986)
C_6H_6-CH_4	0.883	0.00207	-6.180206672
C_6H_6-Ar	0.675	0.00096	-6.948577274
C_6H_6-H_2	0.271	0.000261	-8.250990151
C_6H_6-N_2	0.472	0.00044	-7.728735831
C_6H_6-O_2	0.597	0.000816	-7.111096203
C_6H_6-CO	0.596	0.000663	-7.318735568
C_6H_6-CO_2	1.08	0.00962	-4.643911014
C_6H_6-He	0.132	0.000077	-9.471705136
C_6H_6-SO_2	1.603	0.23	-1.46967597
mixture solvent-solute	**PE(uv) (equation (4.2)) Mohammadi (1986)**	**x_{solute} Mohammadi (1986)**	**ln x_{solute} Mohammadi (1986)**
CCl_4-CH_4	0.801	0.00286	-5.856933654
CCl_4-Ar	0.625	0.00135	-6.607650687
CCl_4-H_2	0.309	0.000327	-8.025550387
CCl_4-N_2	0.432	0.000642	-7.350922254
CCl_4-O_2	0.548	0.0012	-6.725433722
CCl_4-CO	0.547	0.000886	-7.028793607
CCl_4-CO_2	0.976	0.01	-4.605170186
CCl_4-SO_2	1.45	0.15	-1.897119985

Table A4-1. The modified potentials obtained by Mohammadi (1986) for selected mixtures of a series of solutes dissolved in benzene, carbon tetrachloride, and water (continued over).

mixture solvent-solute	PE(uv) (equation (4.2)) Mohammadi (1986)	x_{solute} Mohammadi (1986)	ln x_{solute} Mohammadi (1986)
H_2O-CH_4	3.667	0.000028	-10.48330605
H_2O -Ar	2.342	0.000025	-10.59663473
H_2O -H_2	0.968	0.000014	-11.17645323
H_2O -N_2	1.739	0.0000115	-11.37316352
H_2O -O_2	2.23	0.0000227	-10.69314563
H_2O -CO	2.226	0.000018	-10.9251388
H_2O -CO_2	4.643	0.0007	-7.264430223
H_2O -He	0.458	0.0000067	-11.91340303
H_2O -SO_2	6.844	0.0434	-3.137295838

Table A4-1. The modified potentials obtained by Mohammadi (1986) for selected mixtures of a series of solutes dissolved in benzene, carbon tetrachloride, and water.

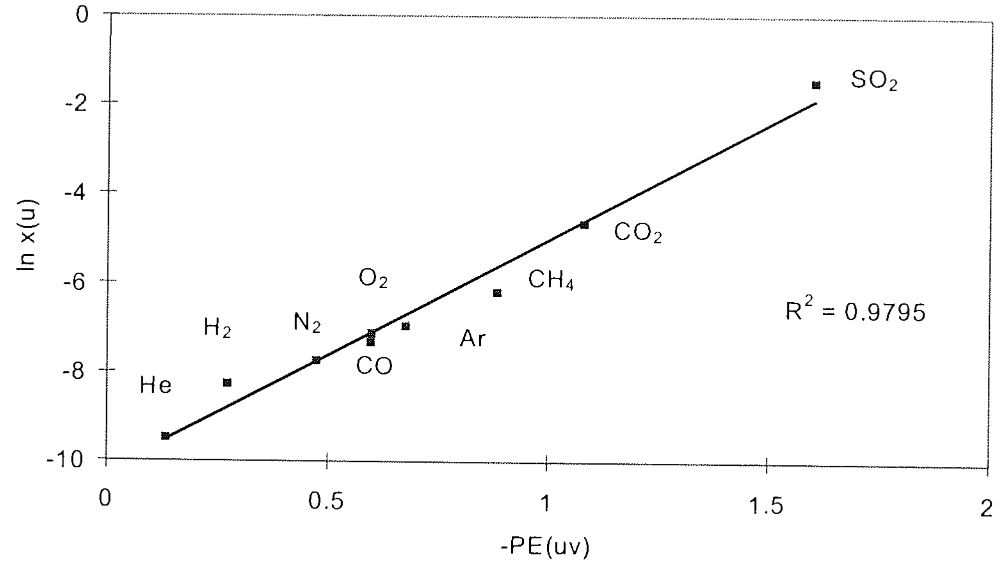

Figure A4.1. Solubilities of gases in **benzene** at 298.15 K, 101.325 kPa as a function of the modified potential (-PE(uv), equation (4.2)).

On the figures in this Appendix, the points represent the values from the relevant table and the line is the best line-fit through the points with R^2 being the linear correlation coefficient.

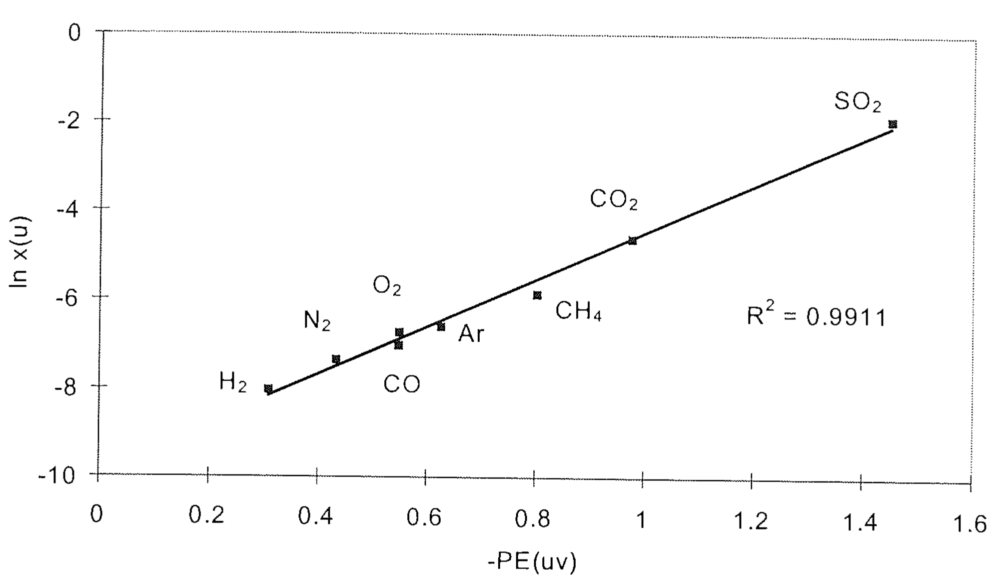

Figure A4.2. Solubilities of gases in **carbon tetrachloride** at 298.15 K, 101.325 kPa as a function of the modified potential (-PE(uv), equation (4.2)).

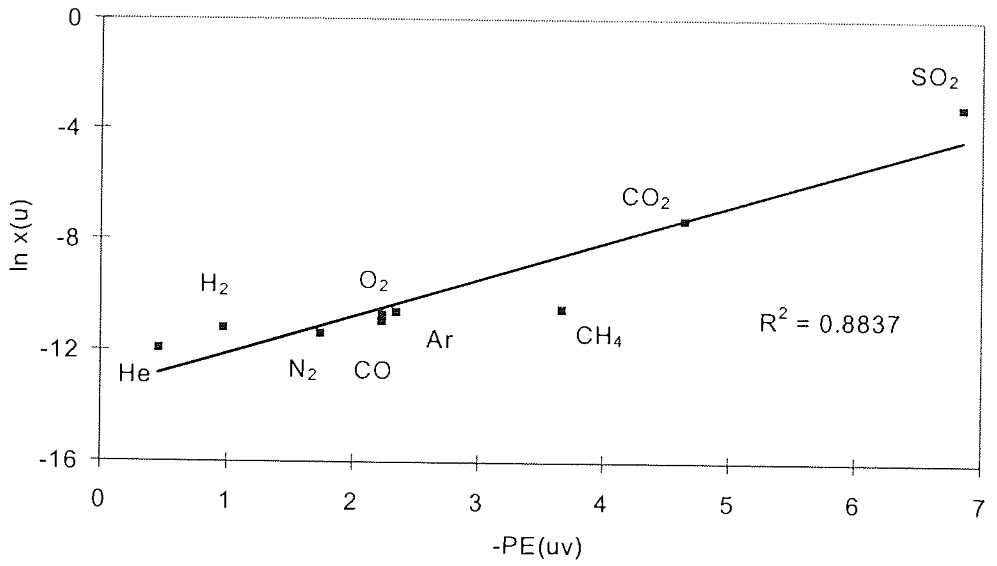

Figure A4.3. Solubilities of gases in **water** at 298.15 K, 101.325 kPa as a function of the modified potential (-PE(uv), equation (4.2)).

Appendix 5 - Results of the VNUN calculation method

A5.1 Results of VNUN calculations for a series of solutes dissolved in a single solvent

All tables in this appendix show the mixture in the first column, then the experimental solubility at 298.15 K and partial pressure of the solute of 101.325 kPa (from Table A3-1), the next column displays the base 10 logarithm of the solubility, then follows the unlike London pair potential for the mixture. For some solvents, another column showing the unlike geometric pair potential follows. In some cases, the geometric mean pair potentials have been calculated and are shown in the table, but not plotted in a graph.

The experimental solubility data are from Fogg and Gerard (1991) or IUPAC Solubility Data Series (Clever, 1979 (vol. 1), Clever, 1980 (vol. 4), Young, 1981 (vol. 5/6), Battino, 1981 (vol. 7), Hayduk, 1982 (vol. 9), Battino, 1982 (vol. 10), Hayduk, 1986 (vol. 24), and Clever and Young, 1987 (vol. 27/28)).

The points on the graphs represent the pair potential, the line is the best fitted straight line through the points and the R^2 is the line correlation coefficient.

VNUN solvent-solute	x_{solute}	log x_{solute}	P12- GLP*E19 (J)	P12- GM*E19 (J)
C_6H_6-CH_4	0.00209	-2.679853714	-4.049400E-02	-4.558000E-02
C_6H_6-Ar	0.000882	-3.054531415	-2.344200E-02	-3.587000E-02
C_6H_6-H_2	0.0002591	-3.586532587	-1.226500E-02	-1.621000E-02
C_6H_6-N_2	0.000445	-3.351639989	-2.060000E-02	-2.613000E-02
C_6H_6-O_2	0.00081	-3.091514981	-2.788100E-02	-3.501600E-02
C_6H_6-CO	0.00065	-3.187086643	-2.225800E-02	-2.780000E-02
C_6H_6-C_2H_4	0.01185	-1.92628165	-4.651900E-02	-4.910000E-02
C_6H_6-C_2H_6	0.0149	-1.826813732	-5.402600E-02	-5.603700E-02
C_6H_6-CO_2	0.00912	-2.040005162	-5.090800E-02	-5.755000E-02
C_6H_6-n-C_3H_8	0.0573	-1.241845378	-8.1338E-02	-8.214059E-02

Table A5-1. The obtained unlike pair potentials calculated by method VNUN and the experimental solubility (x_{solute}) for gases in liquids at 298.15 K, 101.325 kPa (continued over).

VNUN solvent-solute	x_{solute}	**log** x_{solute}	**P12- GLP*E-19 (J)**	**P12- GM*E-19 (J)**
CCl_4-CH_4	0.002856	-2.544241797	-4.811500E-02	-5.228000E-02
CCl_4-Ar	0.00135	-2.869666232	-2.937900E-02	-4.114000E-02
CCl_4-H_2	0.000323	-3.491470281	-1.526300E-02	-1.859000E-02
CCl_4-N_2	0.000641	-3.19314197	-2.545500E-02	-2.996600E-02
CCl_4-O_2	0.0012	-2.920818754	-3.402800E-02	-4.016200E-02
CCl_4-CO	0.000865	-3.062983893	-2.756400E-02	-3.189000E-02
CCl_4-CO_2	0.01	-2	-5.960800E-02	-6.600000E-02
CCl_4-C_2H_4	0.0148	-1.829738285	-5.462600E-02	-5.631500E-02
CCl_4-C_2H_6	0.0211	-1.675717545	-6.288100E-02	-6.427200E-02
CCl_4-n-C_3H_8	0.0813	-1.089909454	-9.0597E-02	-9.4214E-02
CCl_4-n-C_4H_{10}	0.339	-0.469800302	-10.7774E-02	-11.73039E-02
VNUN solvent-solute	$x_{soolute}$	**log** x_{solute}	**P12 - GLP*E19 (J)**	**P12- GM*E19 (J)**
c-C_6H_{12}-CH_4	0.00327	-2.485452247	-5.058600E-02	-5.773700E-02
c-C_6H_{12}-Ar	0.00114	-2.943095149	-2.808300E-02	-4.543170E-02
c-C_6H_{12}-H_2	0.000414	-3.382999659	-1.508200E-02	-2.053130E-02
c-C_6H_{12}-N_2	0.000768	-3.11463878	-2.502300E-02	-3.309430E-02
c-C_6H_{12}-O_2	0.00123	-2.910094889	-3.441900E-02	-4.435400E-02
c-C_6H_{12}-CO	0.000999	-3.000434512	-2.726300E-02	-3.521300E-02
c-C_6H_{12}-C_2H_6	0.0233	-1.632644079	-6.787200E-02	-7.098060E-02
c-C_6H_{12}-CO_2	0.00759	-2.119758224	-6.316000E-02	-7.289300E-02
c-C_6H_{12} - n-C_3H_8	0.091	-1.040958608	-10.2555E-02	-10.40475E-02
VNUN solvent-solute	x_{solute}	**log** x_{solute}	**P12 - GLP*E19 (J)**	
$CHCl_3$ -Ar	0.000592	-3.227678293	-2.690300E-02	
$CHCl_3$ -H_2	0.00022	-3.657577319	-1.396100E-02	
$CHCl_3$ -N_2	0.000445	-3.351639989	-2.316500E-02	
$CHCl_3$ -CO	0.000665	-3.177178355	-2.507900E-02	
$CHCl_3$ -CO_2	0.0128	-1.89279003	-5.437100E-02	
VNUN solute-solvent	x_{solute}	**log** x_{solute}	**P12 -GLP*E19 (J)**	
CS_2 -CH_4	0.001309	-2.883060353	-5.484700E-02	
CS_2 -Ar	0.000486	-3.31309573	-3.530700E-02	
CS_2 -H_2	0.000159	-3.797784224	-1.786600E-02	
CS_2 -N_2	0.000222	-3.654626269	-2.945000E-02	
CS_2 -O_2	0.000439	-3.35753548	-3.982400E-02	
CS_2 -CO	0.00036	-3.443697499	-3.167600E-02	
CS_2 -C_2H_6	0.0107	-1.970616222	-6.936200E-02	
CS_2 -CO_2	0.00328	-2.484126156	-6.886000E-02	
CS_2 -n-C_3H_8	0.0446	-1.350665141	-9.8991E-02	

Table A5-1. The obtained unlike pair potentials calculated by method VNUN and the experimental solubility (x_{solute}) for gases in liquids at 298.15 K, 101.325 kPa (continued over).

VNUN solvent-solute	x_{solute}	log x_{solute}	P12 - GLP*E19 (J)	P12- GM*E19 (J)
H_2O-CH_4	0.00002548	-4.593800576	-5.456900E-02	-6.427400E-02
H_2O-Ar	0.00002519	-4.598771833	-3.538400E-02	-5.057560E-02
H_2O-H_2	0.00001411	-4.850472986	-1.788600E-02	-2.285500E-02
H_2O-N_2	0.00001183	-4.927015255	-2.645100E-02	-3.684000E-02
H_2O-O_2	0.00002293	-4.639595945	-4.115700E-02	-4.937600E-02
H_2O-CO	0.0000172	-4.764471553	-2.868900E-02	-3.920000E-02
H_2O-C_2H_4	0.00008582	-4.06641149	-5.544800E-02	-8.114600E-02
H_2O-C_2H_6	0.000034	-4.468521083	-6.242000E-02	-6.923500E-02
H_2O-CO_2	0.0006116	-3.213532523	-7.101200E-02	-7.901700E-02
H_2O-n-C_3H_8	0.00002732	-4.563519305	-9.1447E-02	-11.58282E-02
H_2O-n-C_4H_{10}	0.00002244	-4.648977147	-11.0854E-02	-14.42154E-02

VNUN solvent-solute	x_{solute}	log x_{solute}	P12-GLP*E19 (J)	P12-GM*E19 (J)
CH_3OH-CH_4	0.000871	-3.059981845	-0.043651	-0.045616236
CH_3OH-Ar	0.000447	-3.349692477	-0.026046	-0.035894172
CH_3OH-H_2	0.000161	-3.793174124	-0.01367	-0.016221136
CH_3OH-N_2	0.000276	-3.559090918	-0.021534	-0.026146775
CH_3OH-O_2	0.000415	-3.381951903	-0.031266	-0.035042678
CH_3OH-CO	0.000327	-3.485452247	-0.023419	-0.027821567
CH_3OH-C_2H_4	0.0047	-2.327902142	-0.047437	-0.049138059
CH_3OH-C_2H_6	0.00393	-2.40560745	-0.054367	-0.056080782
CH_3OH-Ne	0.0000804	-4.094743951	-0.012739	-0.017042405
CH_3OH-n-C_3H_8	0.0115	-1.93930216	-0.080257	-0.082206484
CH_3OH-n-C_4H_{10}	0.0398	-1.400116928	-0.097466	-0.10235365
CH_3OH-CO_2	0.00639	-2.194499142	-0.03761	-0.040595753

VNUN solvent-solute	x_{solute}	log x_{solute}	P12-GLP*E19 (J)	P12-GM*E19 (J)
C_2H_5OH-CH_4	0.00128	-2.89279003	-0.066177	-0.085916901
C_2H_5OH-Ar	0.0006257	-3.203633845	-0.032732	-0.067605665
C_2H_5OH-N_2	0.000357	-3.447331784	-0.028512	-0.049309405
C_2H_5OH-O_2	0.0005825	-3.23470407	-0.043487	-0.0660019
C_2H_5OH-CO	0.000449	-3.347753659	-0.031342	-0.05240004
C_2H_5OH-C_2H_6	0.00666	-2.176525771	-0.086899	-0.105624361
C_2H_5OH-Ne	0.000109	-3.962573502	-0.01619	-0.032098217
C_2H_5OH-H_2	0.000206	-3.68613278	-0.018191	-0.030552054
C_2H_5OH-n-C_3H_8	0.0228	-1.642065153	-0.142497	-0.154830355
C_2H_5OH-n-C_4H_{10}	0.0815	-1.088842391	-0.187243	-0.192776182
C_2H_5OH-CO_2	0.00689	-2.161780778	-0.054984	-0.076459357

Table A5-1. The obtained unlike pair potentials calculated by method VNUN and the experimental solubility (x_{solute}) for gases in liquids at 298.15 K, 101.325 kPa (continued over).

VNUN solvent-solute	x_{solute}	log x_{solute}	P12-GLP*E19 (J)	P12-GM*E19 (J)
C_3H_7OH-CH_4	0.00156	-2.806875402	-0.095048	-0.101750983
C_3H_7OH-Ar	0.000777	-3.109578981	-0.038246	-0.080065073
C_3H_7OH-H_2	0.000231	-3.63638802	-0.022657	-0.036182654
C_3H_7OH-N_2	0.000402	-3.395773947	-0.035009	-0.058322656
C_3H_7OH-O_2	0.000503	-3.298432015	-0.056937	-0.078165741
C_3H_7OH-CO	0.0005193	-3.284581677	-0.03906	-0.062057123
C_3H_7OH-CO_2	0.00772	-2.1123827	-0.12691	-0.128459771

Table A5-1. The obtained unlike pair potentials calculated by method VNUN and the experimental solubility (x_{solute}) for gases in liquids at 298.15 K, 101.325 kPa.

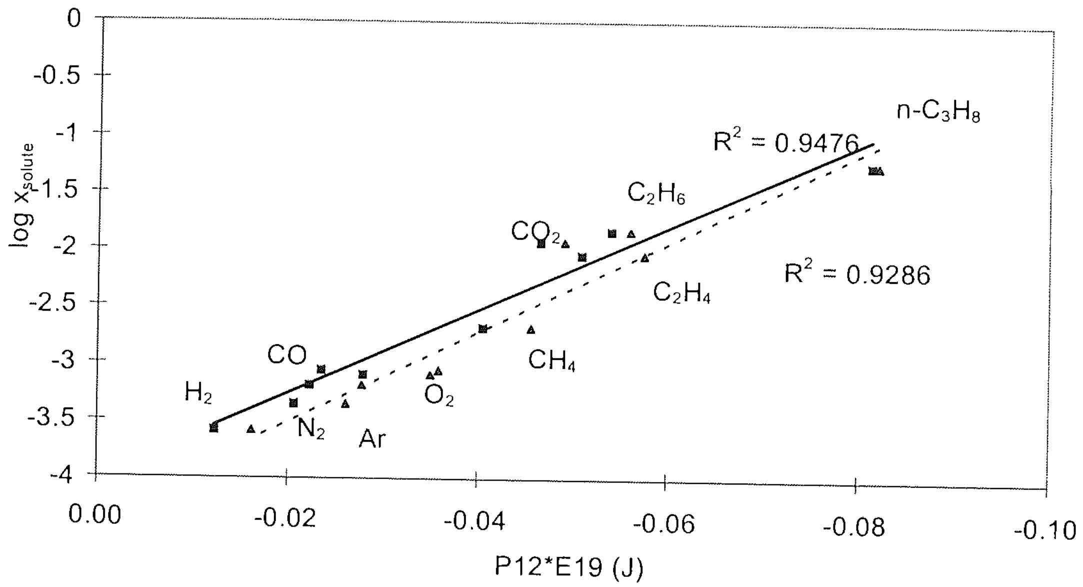

Figure A5.1. Solubilities of gases in **benzene** at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP, ■ points and – line) and the geometric mean unlike pair potential (P12-GM, ▲ points and -- line) calculated by method VNUN.

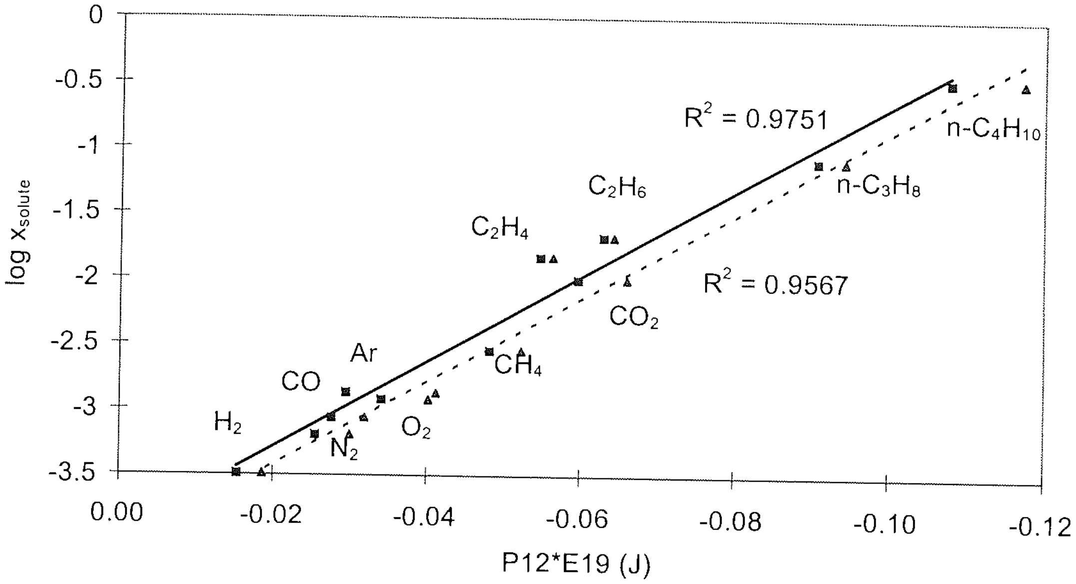

Figure A5.2. Solubilities of gases in **carbon tetrachloride** at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP, ■ points and – line) and the geometric mean unlike pair potential (P12-GM, ▲ points and -- line) calculated by method VNUN.

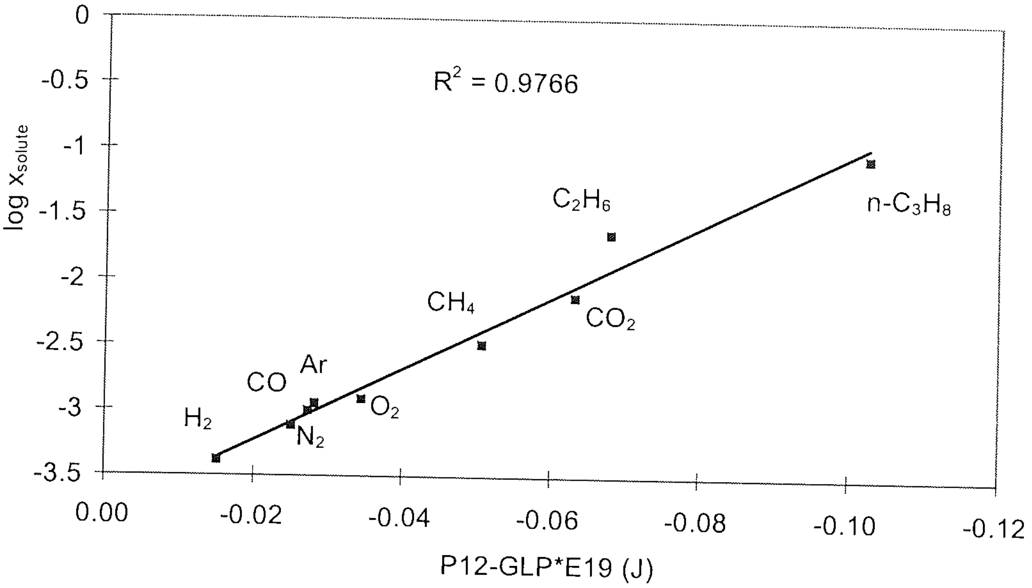

Figure A5.3. Solubilities of gases in ***cyclo* hexane** at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP) calculated by method VNUN.

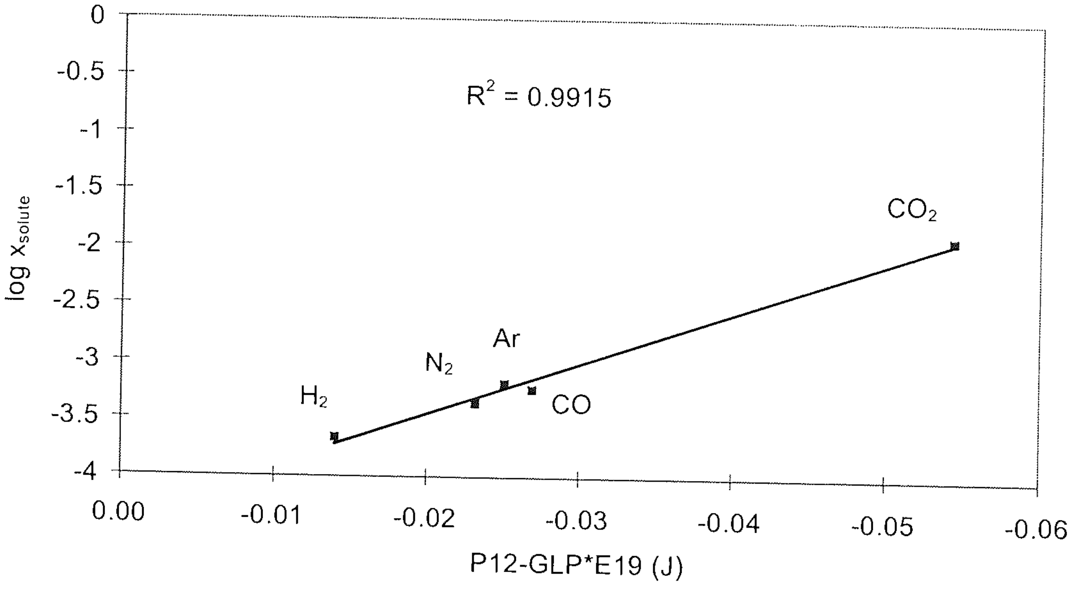

Figure A5.4. Solubilities of gases in **chloroform** at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP) calculated by method VNUN.

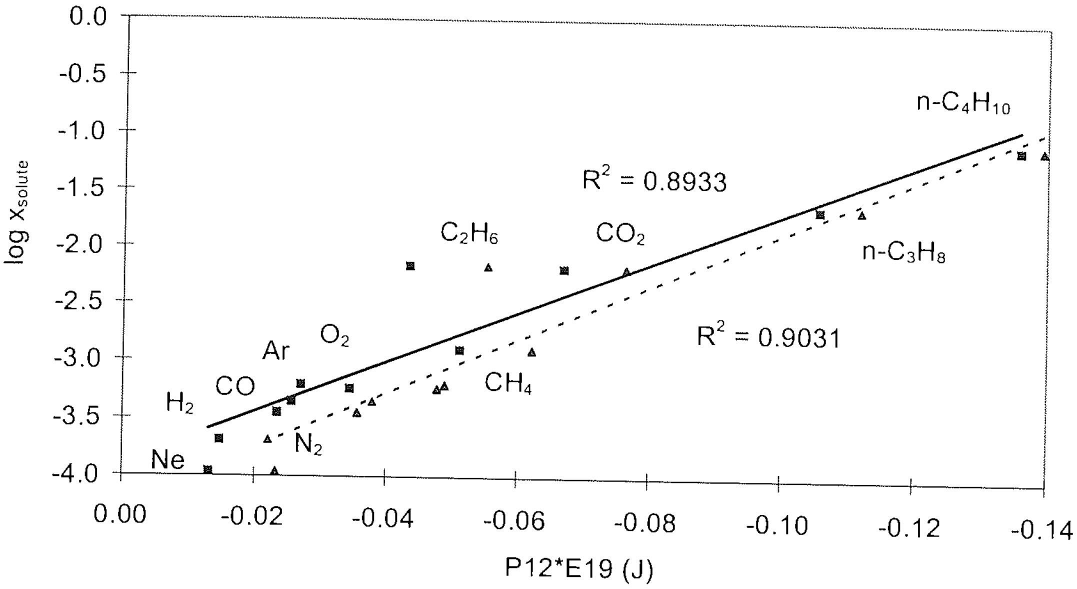

Figure A5.5. Solubilities of gases in **ethanol** at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP, ■ points and — line) and the geometric mean unlike pair potential (P12-GM, ▲ points and -- line) calculated by method VNUN.

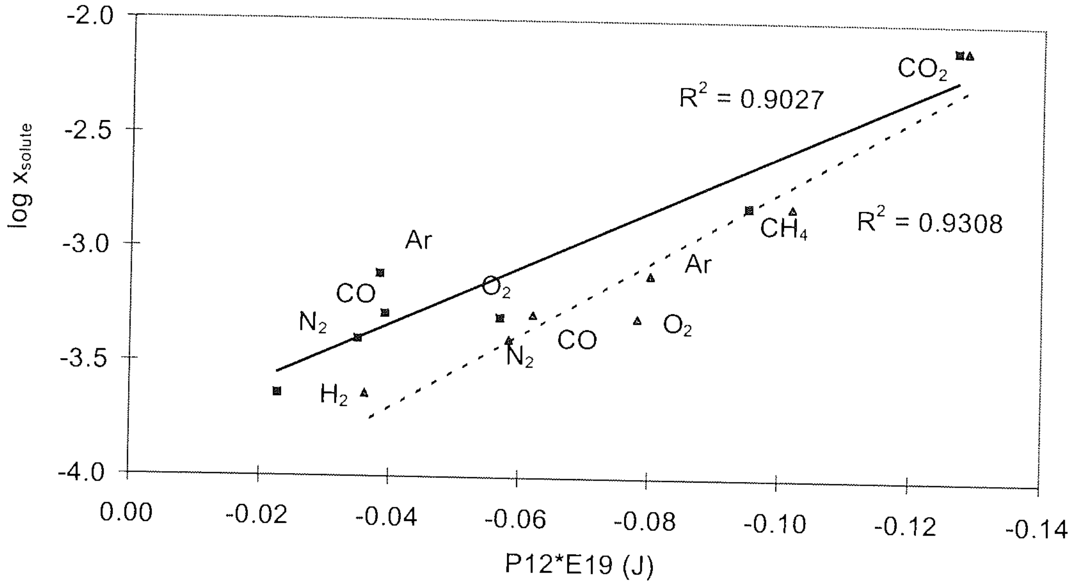

Figure A5.6. Solubilities of gases in **1-propanol** at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP, ■ points and – line) and the geometric mean unlike pair potential (P12-GM, ▲ points and -- line) calculated by method VNUN.

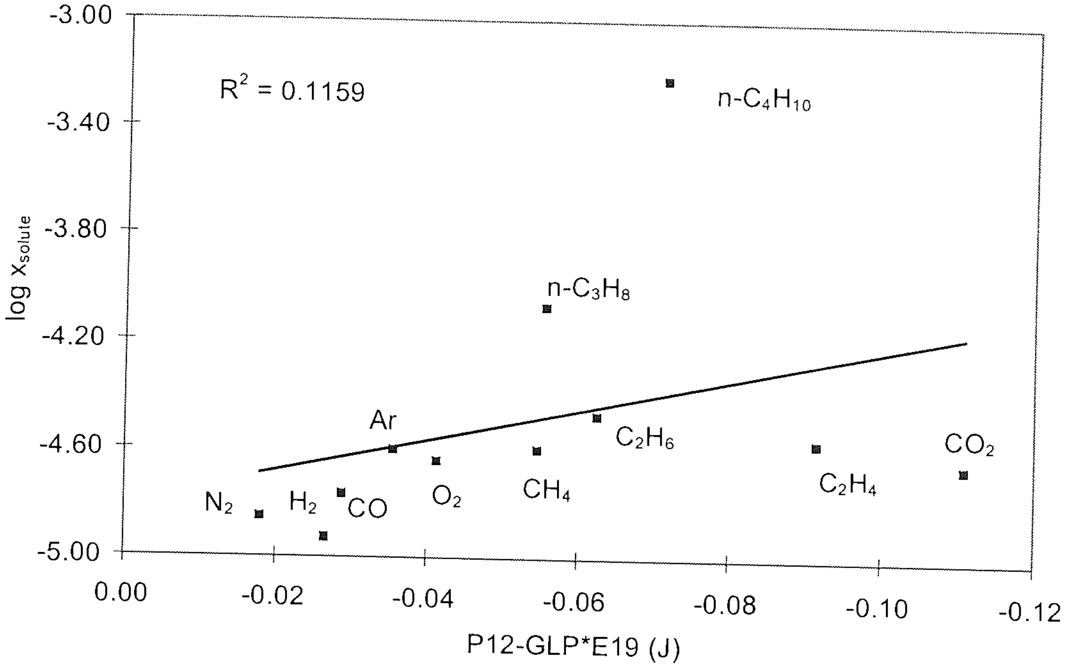

Figure A5.7. Solubilities of gases in **water** at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP) calculated by method VNUN.

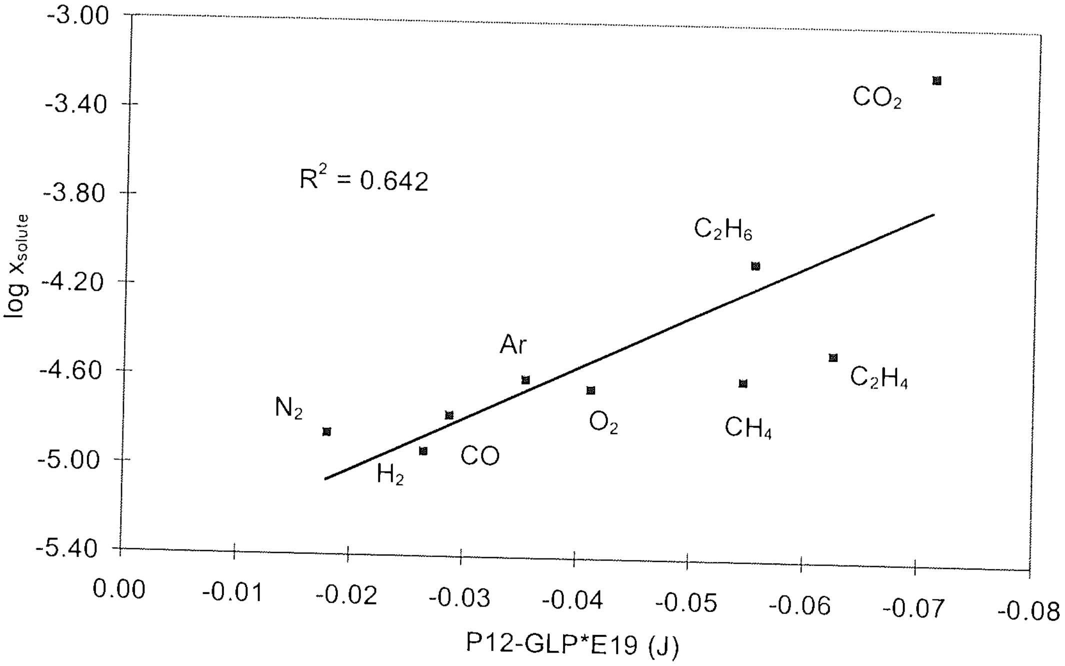

Figure A5.8. Solubilities of gases in **water** at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP) calculated by method VNUN (excluding datapoints for n-propane and n-butane).

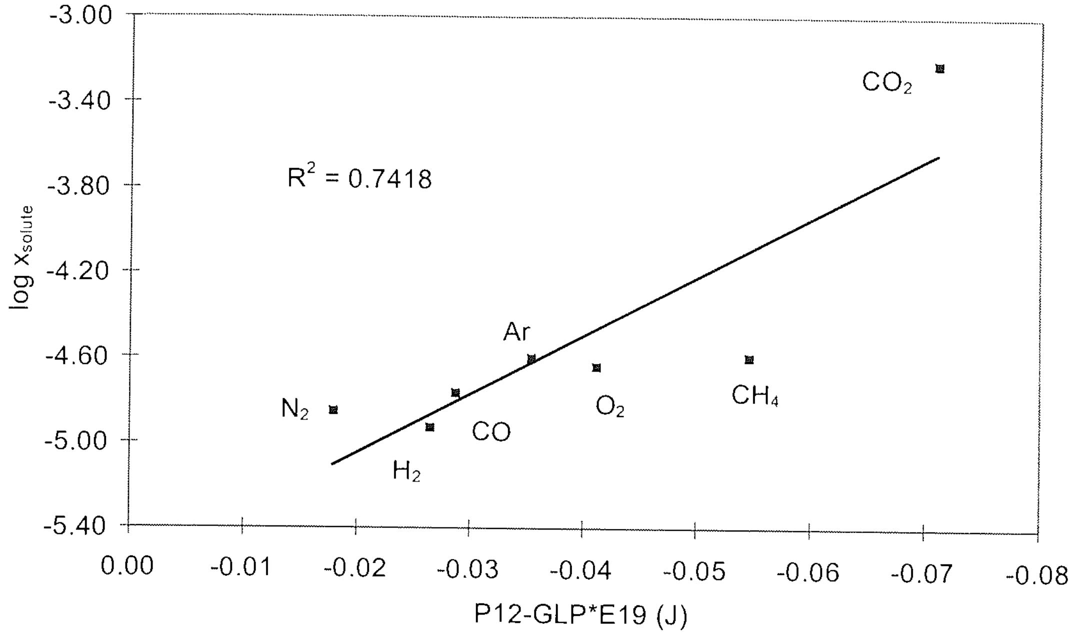

Figure A5.9. Solubilities of gases in **water** at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP) calculated by method VNUN (excluding datapoints for n-propane, n-butane and ethylene).

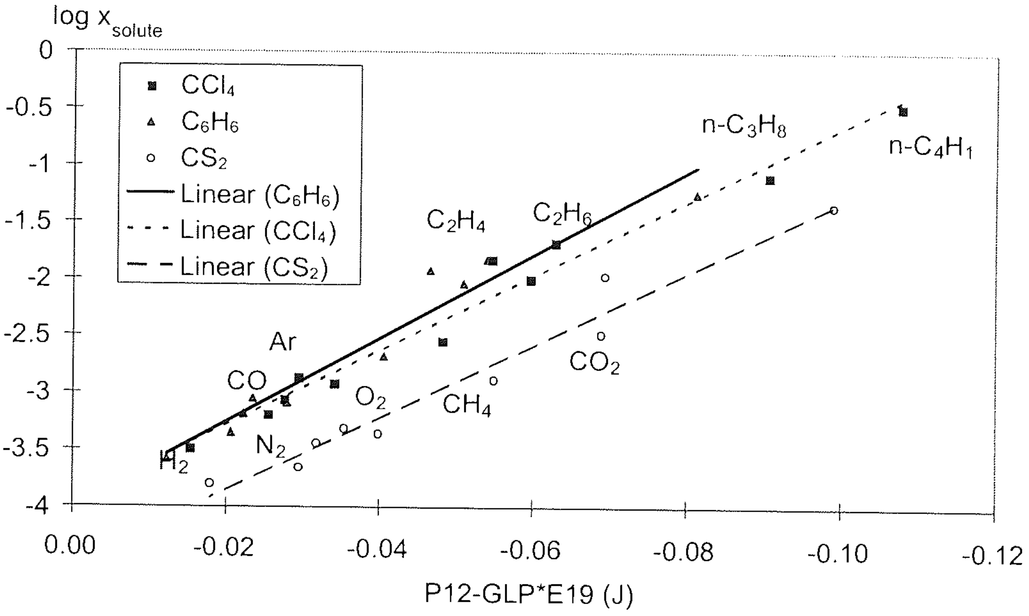

Figure A5.10. Solubilities of gases in **benzene** (▲ and continuos—), **carbon tetrachloride** (■ and --) and **carbon disulfide** (● and — —) at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP) calculated by method VNUN.

A5.2 Results of VNUN calculations for a single solute dissolved in a series of solvents

VNUN solvent-solute	x_{solute}	log x_{solute}	P12-GLP*E19 (J)
C_6H_6-Ar	0.00882	-3.054531415	-2.344200E-02
c-C_6H_{12}-Ar	0.00114	-2.943095149	-2.808300E-02
CCl_4-Ar	0.00135	-2.869666232	-2.937900E-02
CS_2-Ar	0.0004863	-3.31309573	-3.530700E-02
H_2O-Ar	0.00002519	-4.598771833	-3.538400E-02
CH_3OH-Ar	0.000447	-3.349692477	-0.026046
C_2H_5OH-Ar	0.0006257	-3.203633845	-0.032732
C_3H_7OH-Ar	0.000777	-3.109578981	-0.038246
$CHCl_3$-Ar	0.000592	-3.227678293	-2.690300E-02

VNUN solvent-solute	x_{solute}	log x_{solute}	P12-GLP*E19 (J)
C_6H_6-CH_4	0.00209	-2.679853714	-4.049400E-02
c-C_6H_{12}- CH_4	0.00327	-2.485452247	-5.058600E-02
CCl_4- CH_4	0.002856	-2.544241797	-4.811500E-02
CS_2- CH_4	0.001309	-2.883060353	-5.484700E-02
H_2O- CH_4	0.00002548	-4.593800576	-5.456900E-02
CH_3OH- CH_4	0.000871	-3.059981845	-4.3651E-02
C_2H_5OH- CH_4	0.00128	-2.89279003	-6.6177E-02
C_3H_7OH- CH_4	0.00156	-2.804100348	-9.5048E-02

VNUN solvent-solute	x_{solute}	log x_{solute}	P12-GLP*E19 (J)
C_6H_6-n-C_3H_8	0.0573	-1.241845378	-0.081338
c-C_6H_{12}- n-C_3H_8	0.0910	-1.040958608	-0.102555
CCl_4- n-C_3H_8	0.0813	-1.089909454	-0.090597
CS_2- n-C_3H_8	0.0446	-1.350665141	-0.098991
H_2O- n-C_3H_8	0.00002732	-4.563519305	-0.091447
CH_3OH- n-C_3H_8	0.0115	-1.93930216	-0.080257
C_2H_5OH- n-C_3H_8	0.0228	-1.642065153	-0.142497

VNUN solvent-solute	x_{solute}	log x_{solute}	P12-GLP*E19 (J)
C_6H_6-CO_2	0.00912	-2.040005	-5.090800E-02
c-C_6H_{12}-CO_2	0.00759	-2.119758	-6.316000E-02
CCl_4-CO_2	0.0106	-1.9746941	-5.960800E-02
CS_2-CO_2	0.00328	-2.4910665	-6.886000E-02
H_2O-CO_2	0.0006116	-3.2135325	-7.101200E-02
CH_3OH-CO_2	0.00639	-2.1944991	-3.761E-02
C_2H_5OH-CO_2	0.00689	-2.1617808	-5.4984E-02
C_3H_7OH-CO_2	0.00772	-2.1123827	-12.691E-02
$CHCl_3$- CO_2	0.0128	-1.89279003	-5.437100E-02

Table A5-2. The obtained unlike pair potentials calculated by method VNUN and the experimental solubility (x_{solute}) for gases in liquids at 298.15 K, 101.325 kPa (continued over).

VNUN solvent-solute	x_{solute}	log x_{solute}	**P12-GLP*E19 (J)**
C_6H_6-H_2	0.0002591	-3.586532587	-1.226500E-02
c-C_6H_{12}- H_2	0.000414	-3.382999659	-1.508200E-02
CS_2- H_2	0.0001593	-3.797784224	-1.526300E-02
H_2O- H_2	0.00001411	-4.850472986	-1.786600E-02
CCl_4- H_2	0.0003225	-3.491470281	-1.788600E-02
CH_3OH-H_2	0.000161	-3.491470281	-1.367E-02
C_2H_5OH-H_2	0.000206	-3.688246139	-1.8191E-02
C_3H_7OH- H_2	0.000231	-3.63638802	-2.2657E-02
$CHCl_3$- H_2	0.00022	-3.657577319	-1.396100E-02
VNUN solvent-solute	x_{solute}	log x_{solute}	**P12-GLP*E19 (J)**
C_6H_6-N_2	0.000445	-3.351639989	-2.060000E-02
c-C_6H_{12}- N_2	0.000768	-3.11463878	-2.502300E-02
CS_2- N_2	0.0002215	-3.654626269	-2.545500E-02
H_2O- N_2	0.00001183	-4.927015255	-2.945000E-02
CCl_4- N_2	0.000641	-3.19314197	-2.645100E-02
CH_3OH-N_2	0.000276	-3.559090918	-.2.1534E-02
C_2H_5OH-N_2	0.000357	-3.447331784	-2.8512E-02
C_3H_7OH - N_2	0.000402	-3.395773947	-3.5009E-02
$CHCl_3$ - N_2	0.000445	-3.351639989	-2.316500E-02
VNUN solvent-solute	x_{solute}	log x_{solute}	**P12-GLP*E19 (J)**
C_6H_6-O_2	0.000810	-3.091514981	-2.788100E-02
c-C_6H_{12}- O_2	0.00123	-2.910094889	-3.441900E-02
CS_2- O_2	0.000439	-3.35753548	-3.402800E-02
H_2O- O_2	0.00002293	-4.639595945	-3.982400E-02
CCl_4- O_2	0.0012	-2.920818754	-4.115700E-02
CH_3OH-O_2	0.000415	-3.381951903	-0.031266
C_2H_5OH-O_2	0.0005825	-3.23470407	-0.043487
C_3H_7OH - O_2	0.000503	-3.298432015	-0.056937
VNUN solvent-solute	x_{solute}	log x_{solute}	**P12-GLP*E19 (J)**
C_6H_6-CO	0.00065	-3.187086643	-2.225800E-02
c-C_6H_{12}- CO	0.00099	-3.000434512	-2.726300E-02
CS_2- CO	0.00036	-3.443697499	-2.756400E-02
H_2O- CO	0.0000172	-4.764471553	-3.167600E-02
CCl_4- CO	0.000865	-3.062983893	-2.868900E-02
CH_3OH-CO	0.000327	-3.485452247	-0.031266
C_2H_5OH-CO	0.000449	-3.347753659	-0.031342
C_3H_7OH - CO	0.0005193	-3.284581677	-0.03906
$CHCl_3$ - CO	0.000665	-7.31572	-2.507900E-02

Table A5-2. The obtained unlike pair potentials calculated by method VNUN and the experimental solubility (x_{solute}) for gases in liquids at 298.15 K, 101.325 kPa (continued over).

VNUN solvent-solute	x_{solute}	**log x_{solute}**	**P12-GLP*E19 (J)**
C_6H_6-C_2H_6	0.0149	-1.826813732	-5.402600E-02
c-C_6H_{12}- C_2H_6	0.0233	-1.632644079	-6.787200E-02
CS_2- C_2H_6	0.0107	-1.970616222	-6.288100E-02
H_2O- C_2H_6	0.000034	-4.468521083	-6.936200E-02
CCl_4- C_2H_6	0.0211	-1.675717545	-6.242000E-02
CH_3OH-C_2H_6	0.00393	-2.40560745	-0.047437
C_2H_5OH-C_3H_6	0.0666	-2.176525771	-0.086899

Table A5-2. The obtained unlike pair potentials calculated by method VNUN and the experimental solubility (x_{solute}) for gases in liquids at 298.15 K, 101.325 kPa.

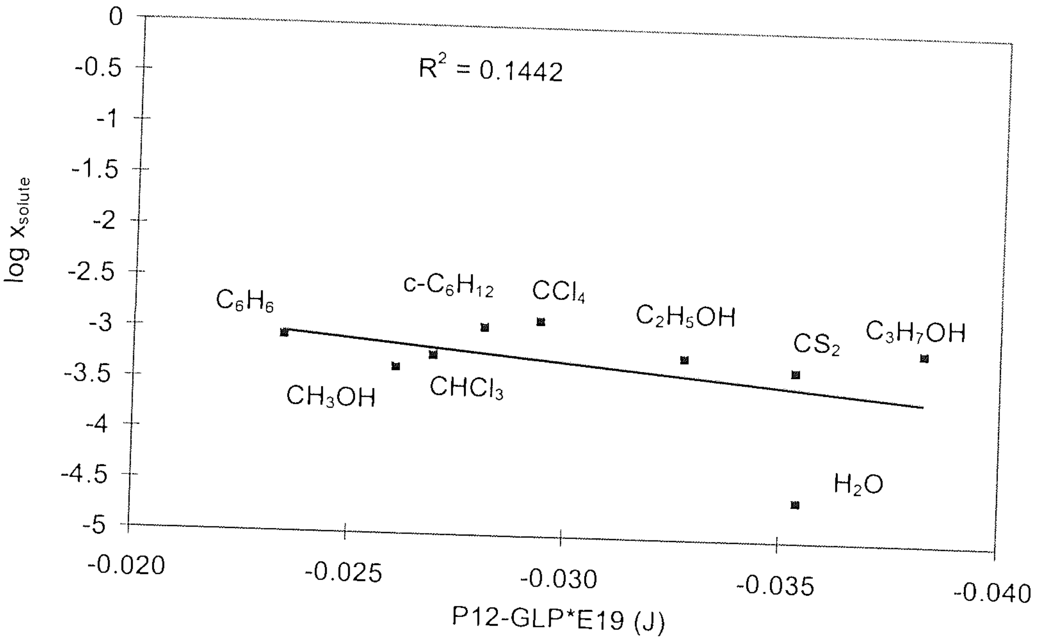

Figure A5.11. Solubilities of **argon** in solvents at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP) calculated by method VNUN.

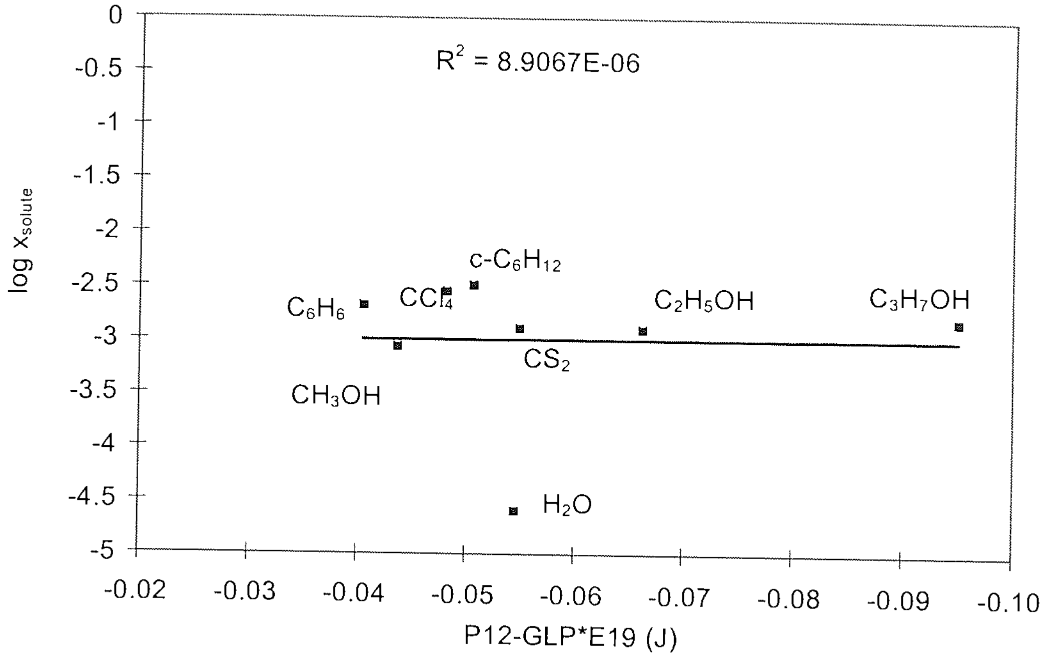

Figure A5.12. Solubilities of **methane** in solvents at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP) calculated by method VNUN.

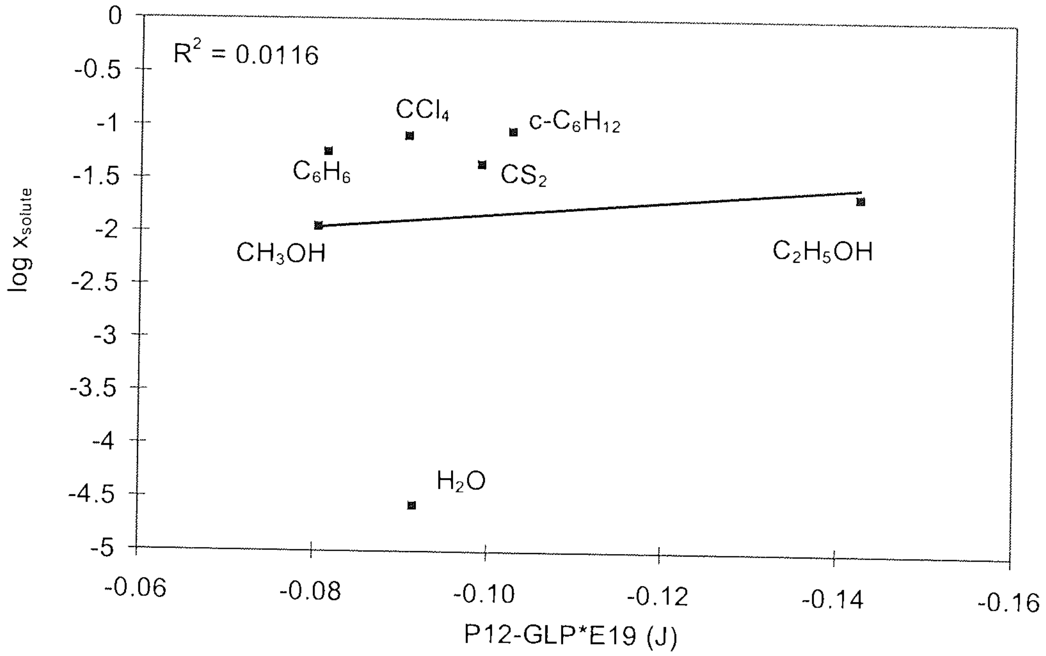

Figure A5.13. Solubilities of **n-propane** in solvents at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP) calculated by method VNUN.

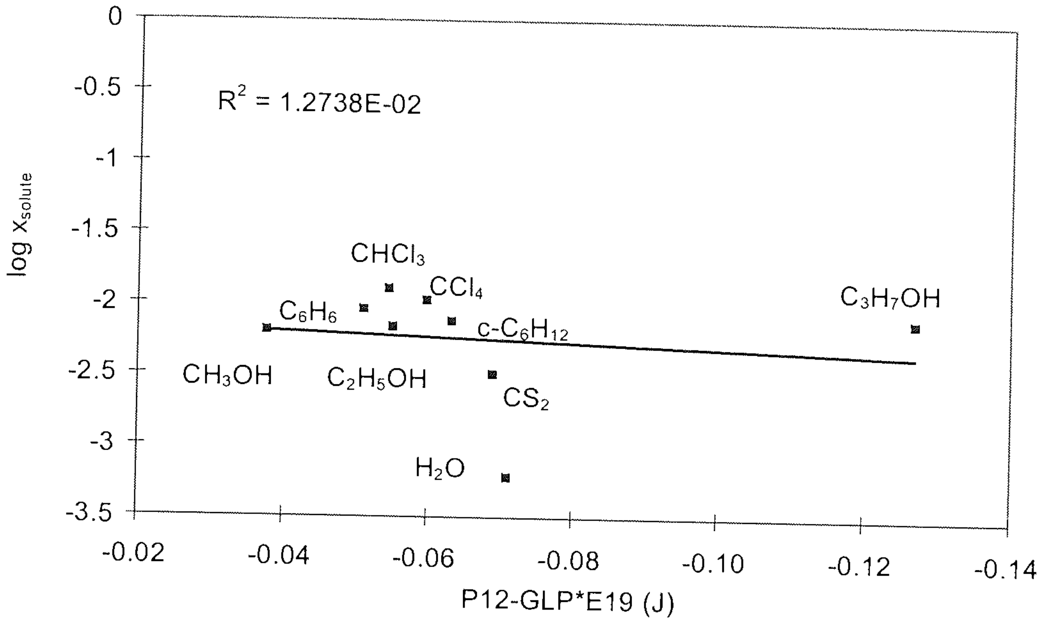

Figure A5.14. Solubilities of **carbon dioxide** in solvents at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP) calculated by method VNUN.

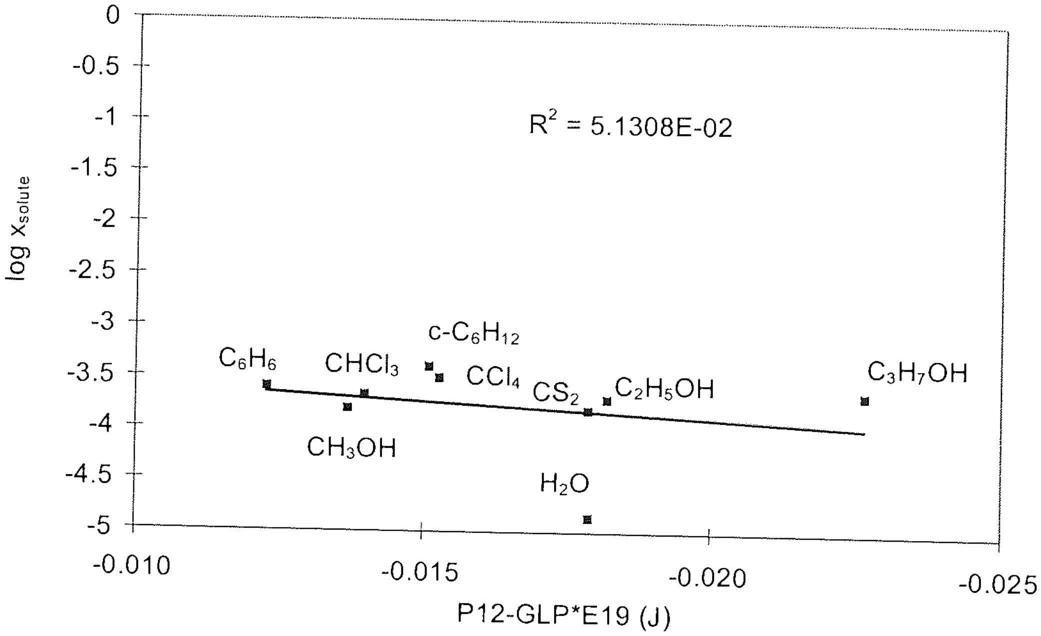

Figure A5.15. Solubilities of **hydrogen** in solvents at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP) calculated by method VNUN.

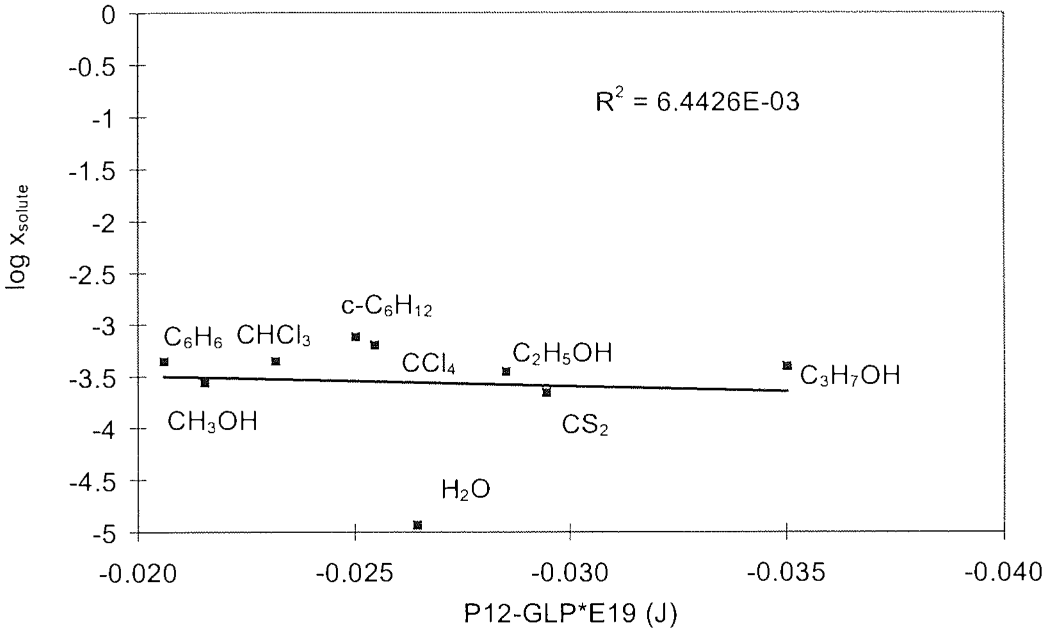

Figure A5.16. Solubilities of **nitrogen** in solvents at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP) calculated by method VNUN.

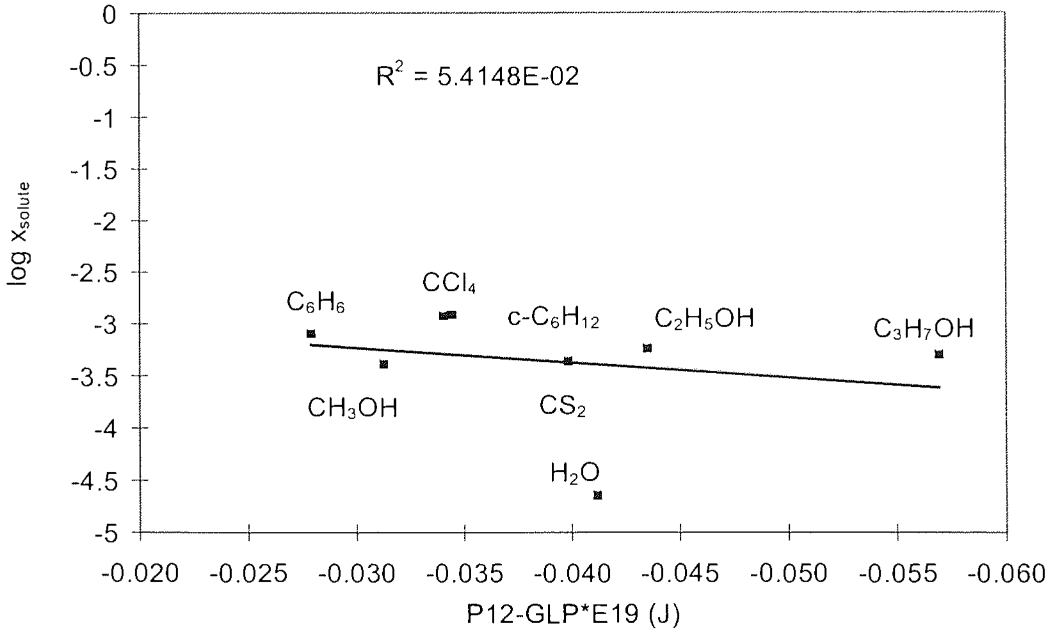

Figure A5.17. Solubilities of **oxygen** in solvents at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP) calculated by method VNUN.

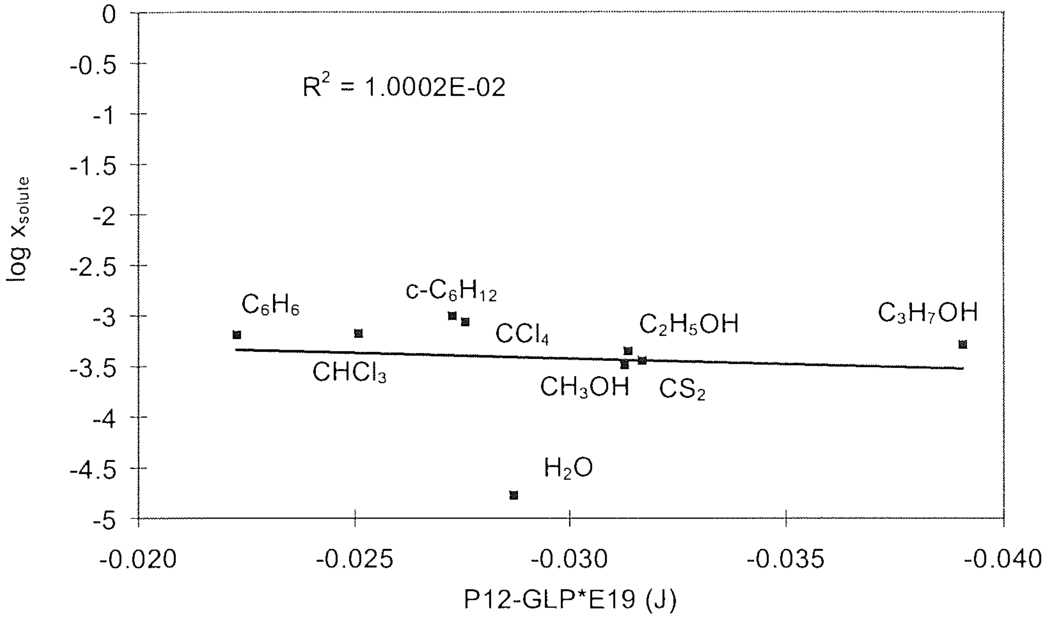

Figure A5.18. Solubilities of **carbon monoxide** in solvents at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP) calculated by method VNUN.

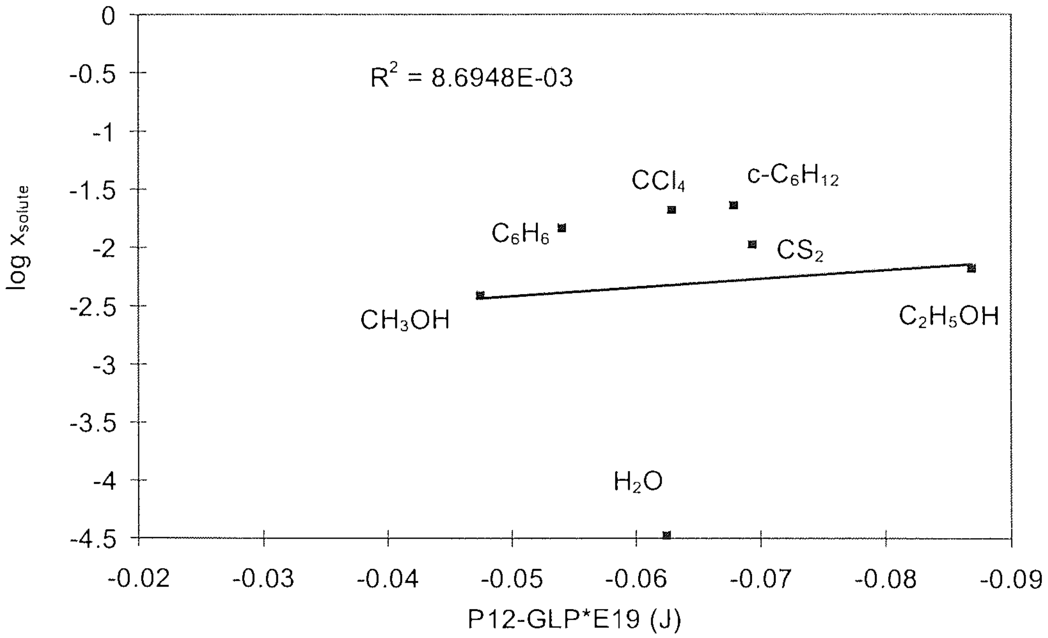

Figure A5.19. Solubilities of **ethane** in solvents at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP) calculated by method VNUN.

Appendix 6 - Results of the VDUN calculation method

All tables in this appendix show the mixture in the first column, then the experimental solubility at 298.15 K and partial pressure of the solute of 101.325 kPa (from Table A3-1), the next column displays the base 10 logarithm of the solubility, then follows the unlike London pair potential for the mixture. For some solvents, another column showing the unlike geometric pair potential follows. In some cases, the geometric mean pair potentials have been calculated and are shown in the table, but not plotted in a graph.

The experimental solubility data are from Fogg and Gerard (1991) or IUPAC Solubility Data Series (Clever, 1979 (vol. 1), Clever, 1980 (vol. 4), Young, 1981 (vol. 5/6), Battino, 1981 (vol. 7), Hayduk, 1982 (vol. 9), Battino, 1982 (vol. 10), Hayduk, 1986 (vol. 24), and Clever and Young, 1987 (vol. 27/28)).

The points on the graphs represent the pair potential, the line is the best fitted straight line through the points and the R^2 is the line correlation coefficient.

A6.1 Results of VDUN calculations for a series of solutes dissolved in a single solvent

VDUN solvent-solute	x_{solute}	log x_{solute}	**P12- GLP*E19 (J)**	**P12- GM*E19 (J)**
C_6H_6-CH_4	0.00209	-2.679853714	-5.181400E-02	-6.003600E-02
C_6H_6-H_2	0.000259	-3.586532587	-1.520300E-02	-2.135000E-02
C_6H_6-N_2	0.000445	-3.351639989	-2.516200E-02	-3.441200E-02
C_6H_6-O_2	0.00081	-3.091514981	-3.511400E-02	-4.612000E-02
C_6H_6-CO_2	0.00912	-2.040005162	-6.571100E-02	-7.579500E-02
C_6H_6-CO	0.00065	-3.187086643	-2.729800E-02	-3.662000E-02
C_6H_6-Ar	0.000882	-3.054531415	-4.001800E-02	-6.733100E-02
C_6H_6-C_2H_4	0.01185	-1.92628165	-5.949800E-02	-6.467000E-02
C_6H_6-C_2H_6	0.0149	-1.826813732	-6.924300E-02	-7.380700E-02
C_6H_6-n-C_3H_8	0.0573	-1.241845378	-10.6985E-02	-10.81904E-02

Table A6-1. The obtained unlike pair potentials calculated by method VDUN and the experimental solubility (x_{solute}) for gases in liquids at 298.15 K, 101.325 kPa (continued over).

VDUN solvent-solute	x_{solute}	log x_{solute}	P12- GLP*E-19 (J)	P12- GM*E-19 (J)
CCl_4-CH_4	0.002856	-2.544241797	-4.280100E-02	-4.696000E-02
CCl_4-Ar	0.00135	-2.869666232	-2.653100E-02	-3.694800E-02
CCl_4-H_2	0.000323	-3.491470281	-1.369300E-02	-1.669740E-02
CCl_4-N_2	0.000641	-3.19314197	-2.289400E-02	-2.691400E-02
CCl_4-O_2	0.0012	-2.920818754	-3.036000E-02	-3.607200E-02
CCl_4-CO	0.000865	-3.062983893	-2.485100E-02	-2.863800E-02
CCl_4-CO_2	0.01	-2	-5.289300E-02	-5.928100E-02
CCl_4-C_2H_4	0.0148	-1.829738285	-4.871600E-02	-5.058000E-02
CCl_4-C_2H_6	0.0211	-1.675717545	-5.598800E-02	-5.772600E-02
CCl_4-n-C_3H_8	0.0813	-1.089909454	-8.016E-02	-8.46183E-02
CCl_4-n-C_4H_{10}	0.339	-0.469800302	-9.4948E-02	-10.532565E-02

VDUN solvent-solute	x_{solute}	log x_{solute}	P12 - GLP*E19 (J)	P12-GM*E19 (J)
c-C_6H_{12}-CH_4	0.00327	-2.485452247	-4.702500E-02	-5.354400E-02
c-C_6H_{12}-Ar	0.00114	-2.943095149	-2.645700E-02	-4.213250E-02
c-C_6H_{12}-H_2	0.000414	-3.382999659	-1.413600E-02	-1.904030E-02
c-C_6H_{12}-N_2	0.000768	-3.11463878	-2.355300E-02	-3.069100E-02
c-C_6H_{12}-O_2	0.00123	-2.910094889	-3.212100E-02	-4.113300E-02
c-C_6H_{12}-CO	0.000999	-3.000434512	-2.563300E-02	-3.265620E-02
c-C_6H_{12}-C_2H_6	0.0233	-1.632644079	-6.308200E-02	-6.582600E-02
c-C_6H_{12}-CO_2	0.00759	-2.119758224	-5.858000E-02	-6.759920E-02
c-C_6H_{12} - n-C_3H_8	0.091	-1.040958608	-9.4695E-02	-9.6492-02

VDUN solvent-solute	x_{solute}	log x_{solute}	P12 - GLP*E19 (J)
$CHCl_3$ -Ar	0.000592	-3.227678293	-2.287500E-02
$CHCl_3$ -H_2	0.00022	-3.657577319	-1.175000E-02
$CHCl_3$ -N_2	0.000445	-3.351639989	-1.969800E-02
$CHCl_3$ -CO	0.000665	-3.177178355	-2.127700E-02
$CHCl_3$ -CO_2	0.0128	-1.89279003	-4.499700E-02

VDUN solvent-solute	x_{solute}	log x_{solute}	P12-GLP*E19 (J)
CS_2 -CH_4	0.001309	-2.883060353	-5.019400E-02
CS_2 -Ar	0.000486	-3.31309573	-3.267200E-02
CS_2 -H_2	0.000159	-3.797784224	-1.671100E-02
CS_2 -N_2	0.000222	-3.654626269	-2.726200E-02
CS_2 -O_2	0.000439	-3.35753548	-3.652300E-02
CS_2 -CO	0.00036	-3.443697499	-2.929200E-02
CS_2 -C_2H_6	0.0107	-1.970616222	-6.353300E-02
CS_2 -CO_2	0.00328	-2.484126156	-6.288300E-02
CS_2 -n-C_3H_8	0.0446	-1.350665141	-9.0205E-02

Table A6-1. The obtained unlike pair potentials calculated by method VDUN and the experimental solubility (x_{solute}) for gases in liquids at 298.15 K, 101.325 kPa (continued over).

VDUN solvent-solute	x_{solute}	log x_{solute}	P12 - GLP*E19 (J)	P12- GM*E19 (J)
H_2O-CH_4	0.00002548	-4.593800576	-2.906100E-02	-2.975100E-02
H_2O-Ar	0.00002519	-4.598771833	-2.036300E-02	-2.341100E-02
H_2O-H_2	0.00001411	-4.850472986	-9.993000E-03	-1.058000E-02
H_2O-N_2	0.00001183	-4.927015255	-1.541400E-02	-1.705300E-02
H_2O-O_2	0.00002293	-4.639595945	-2.226600E-02	-2.285500E-02
H_2O-CO	0.0000172	-4.764471553	-1.659300E-02	-1.814500E-02
H_2O-C_2H_4	0.00008582	-4.06641149	-2.999100E-02	-3.756100E-02
H_2O-C_2H_6	0.000034	-4.468521083	-3.356800E-02	-3.204800E-02
H_2O-CO_2	0.0006116	-3.213532523	-3.702900E-02	-3.657600E-02
H_2O-n-C_3H_8	0.00002732	-4.563519305	-4.6787E-02	-5.36149-02
H_2O-n-C_4H_{10}	0.00002244	-4.648977147	-5.4225E-02	-6.67548-02

VDUN solvent-solute	x_{solute}	log x_{solute}	P12-GLP*E19 (J)	P12-GM*E19 (J)
CH_3OH-CH_4	0.000871	-3.059981845	-0.036225	-0.037122722
CH_3OH-Ar	0.000447	-3.349692477	-0.02224	-0.029210857
CH_3OH-H_2	0.000161	-3.793174124	-0.011542	-0.013200842
CH_3OH-N_2	0.000276	-3.559090918	-0.018393	-0.021278377
CH_3OH-O_2	0.000415	-3.381951903	-0.026131	-0.028517907
CH_3OH-CO	0.000327	-3.485452247	-0.019951	-0.022640856
CH_3OH-C_2H_4	0.0047	-2.327902142	-0.039488	-0.03998796
CH_3OH-C_2H_6	0.00393	-2.40560745	-0.045173	-0.045637864
CH_3OH-Ne	0.0000804	-4.094743951	-0.010707	-0.013868903
CH_3OH-n-C_3H_8	0.0115	-1.93930216	-0.065684	-0.066898646
CH_3OH-n-C_4H_{10}	0.0398	-1.400116928	-0.078747	-0.083294167
CH_3OH-CO_2	0.00639	-2.194499142	-0.031563	-0.033036335

VDUN solvent-solute	x_{solute}	log x_{solute}	P12-GLP*E19 (J)	P12-GM*E19 (J)
C_2H_5OH-CH_4	0.00128	-2.89279003	-0.051052	-0.062118008
C_2H_5OH-Ar	0.0006257	-3.203633845	-0.026916	-0.048878966
C_2H_5OH-N_2	0.000357	-3.447331784	-0.023322	-0.035605427
C_2H_5OH-O_2	0.0005825	-3.23470407	-0.034335	-0.047719442
C_2H_5OH-CO	0.000449	-3.347753659	-0.025539	-0.037885284
C_2H_5OH-C_2H_6	0.00666	-2.176525771	-0.066803	-0.076366523
C_2H_5OH-Ne	0.000109	-3.962573502	-0.01302	-0.023207044
C_2H_5OH-H_2	0.000206	-3.68613278	-0.014652	-0.022089166
C_2H_5OH-n-C_3H_8	0.0228	-1.642065153	-0.105599	-0.111942507
C_2H_5OH-n-C_4H_{10}	0.0815	-1.088842391	-0.135849	-0.139377379
C_2H_5OH-CO_2	0.00689	-2.161780778	-0.043312	-0.055280195

Table A6-1. The obtained unlike pair potentials calculated by method VDUN and the experimental solubility (x_{solute}) for gases in liquids at 298.15 K, 101.325 kPa (continued over).

VDUN solvent-solute	x_{solute}	log x_{solute}	P12-GLP*E19 (J)	P12-GM*E19 (J)
C_3H_7OH-CH_4	0.00156	-2.806875402	-0.06861	-0.077184512
C_3H_7OH-Ar	0.000777	-3.109578981	-0.030687	-0.060734386
C_3H_7OH-H_2	0.000231	-3.63638802	-0.017626	-0.027446816
C_3H_7OH-N_2	0.000402	-3.395773947	-0.027811	-0.044241398
C_3H_7OH-O_2	0.000503	-3.298432015	-0.042913	-0.059293624
C_3H_7OH-CO	0.0005193	-3.284581677	-0.030808	-0.047074225
C_3H_7OH-CO_2	0.00772	-2.1123827	-0.089452	-0.09744409

Table A6-1. The obtained unlike pair potentials calculated by method VDUN and the experimental solubility (x_{solute}) for gases in liquids at 298.15 K, 101.325 kPa.

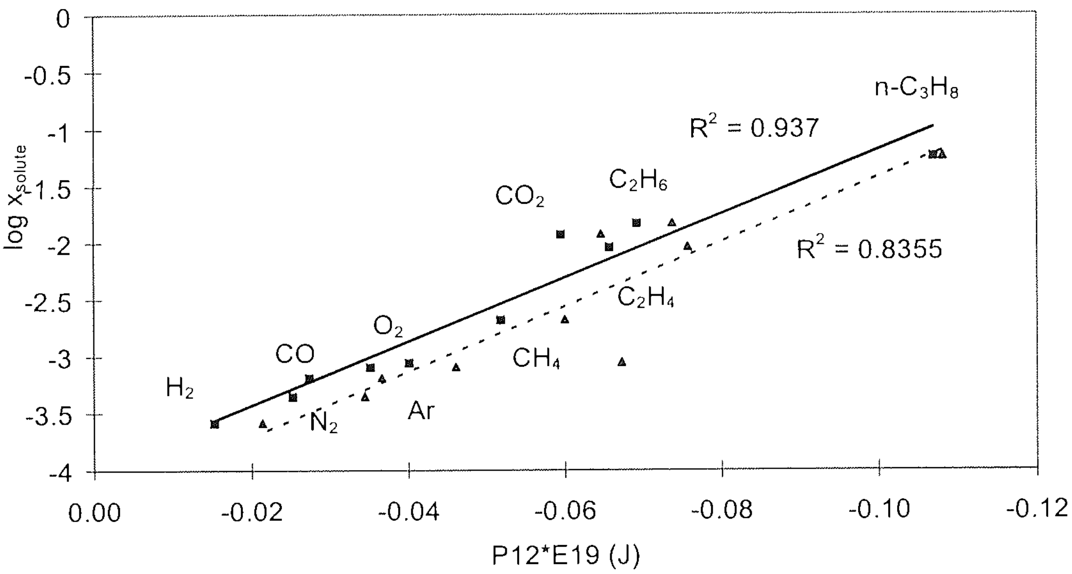

Figure A6.1. Solubilities of gases in **benzene** at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP, ■ points and – line) and the geometric mean unlike pair potential (P12-GM, ▲ points and -- line) calculated by method VDUN.

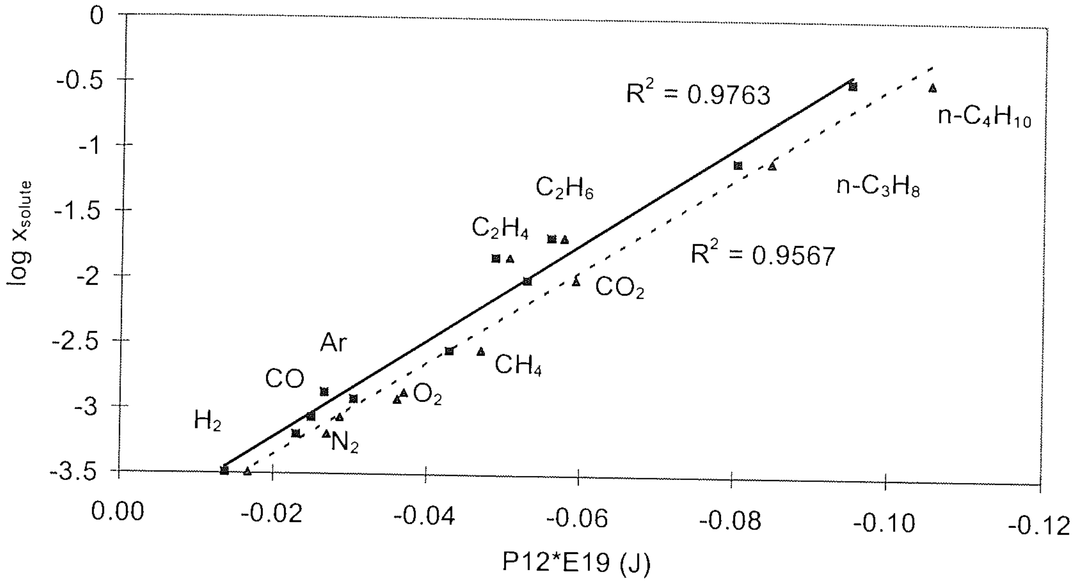

Figure A6.2. Solubilities of gases in **carbon tetrachloride** at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP, ■ points and – line) and the geometric mean unlike pair potential (P12-GM, ▲ points and -- line) calculated by method VDUN.

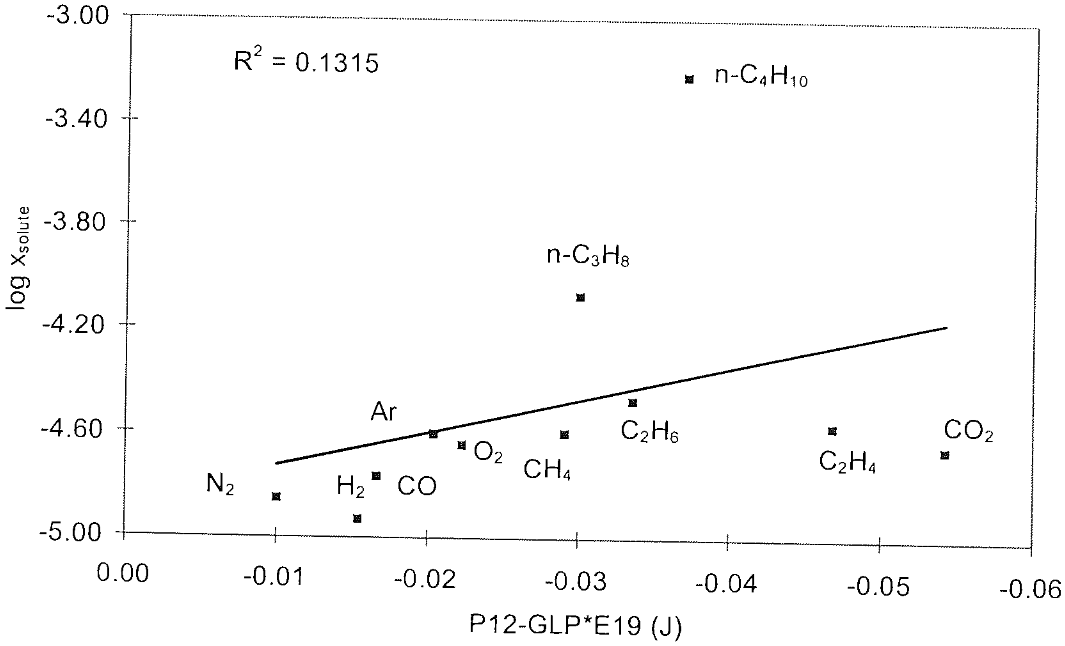

Figure A6.3. Solubilities of gases in **water** at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP) calculated by method VDUN.

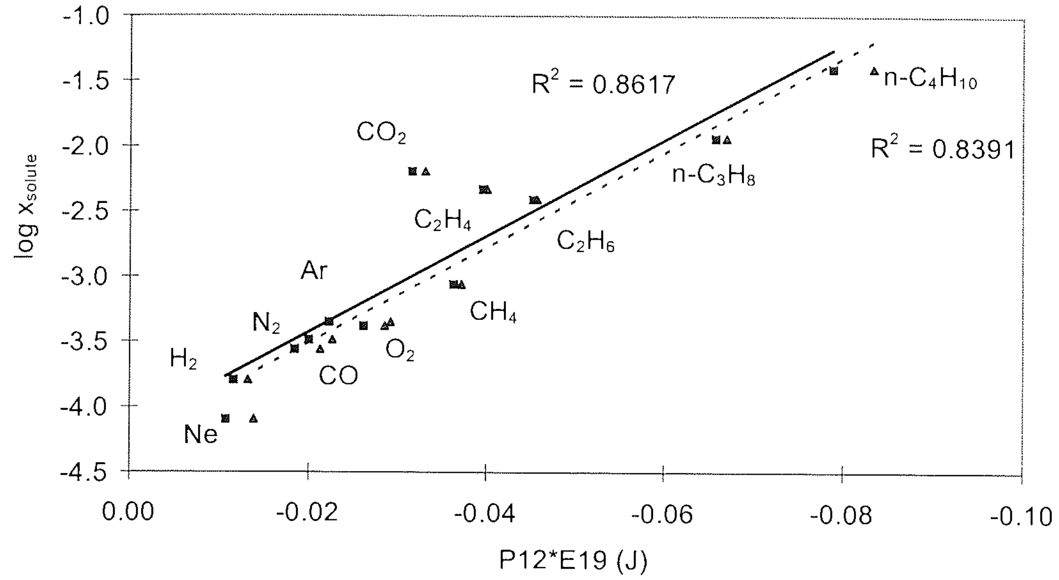

Figure A6.4. Solubilities of gases in **methanol** at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP, ■ points and – line) and the geometric mean unlike pair potential (P12-GM, ▲ points and -- line) calculated by method VDUN.

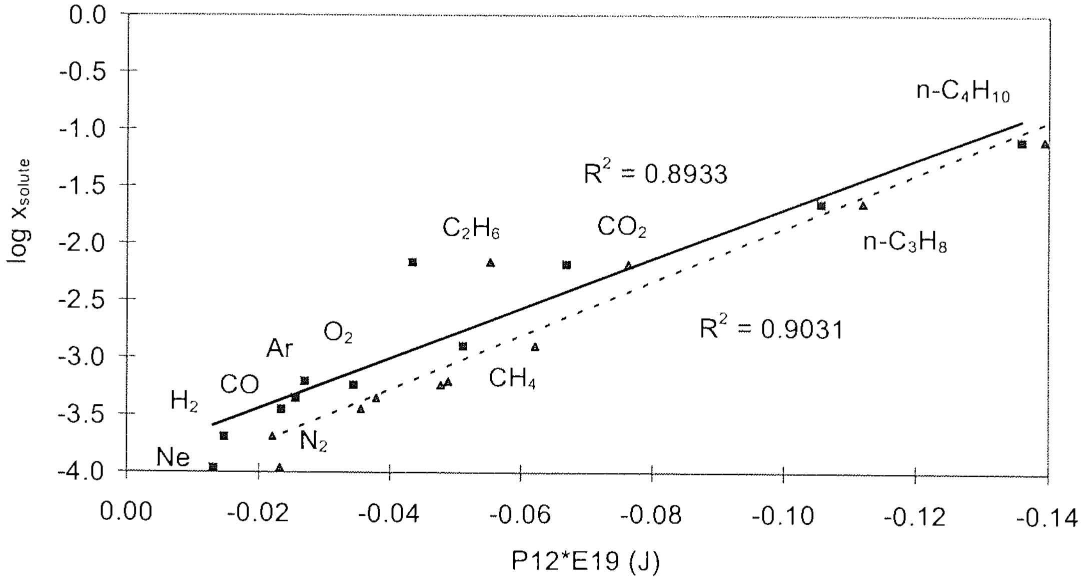

Figure A6.5. Solubilities of gases in **ethanol** at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP, ■ points and – line) and the geometric mean unlike pair potential (P12-GM, ▲ points and -- line) calculated by method VDUN.

A6.2 Results of VDUN calculations for a single solute dissolved in a series of solvents

VDUN solvent-solute	x_{solute}	log x_{solute}	P12-GLP*E19 (J)
C_6H_6-CH_4	0.00209	-2.679853714	-5.181400E-02
c-C_6H_{12}-CH_4	0.00327	-2.485452247	-4.702500E-02
CCl_4-CH_4	0.002856	-2.544241797	-4.280100E-02
CS_2-CH_4	0.001309	-2.883060353	-5.019400E-02
H_2O-CH_4	0.00002548	-4.593800576	-2.906100E-02
CH_3OH-CH_4	0.000871	-3.059981845	-3.6225E-02
C_2H_5OH-CH_4	0.00128	-2.89279003	-5.1052E-02
C_3H_7OH-CH_4	0.00156	-2.804100348	-2.911E-02

Table A6-2. The obtained unlike pair potentials calculated by method VDUN and the experimental solubility (x_{solute}) for **methane** in liquids at 298.15 K, 101.325 kPa.

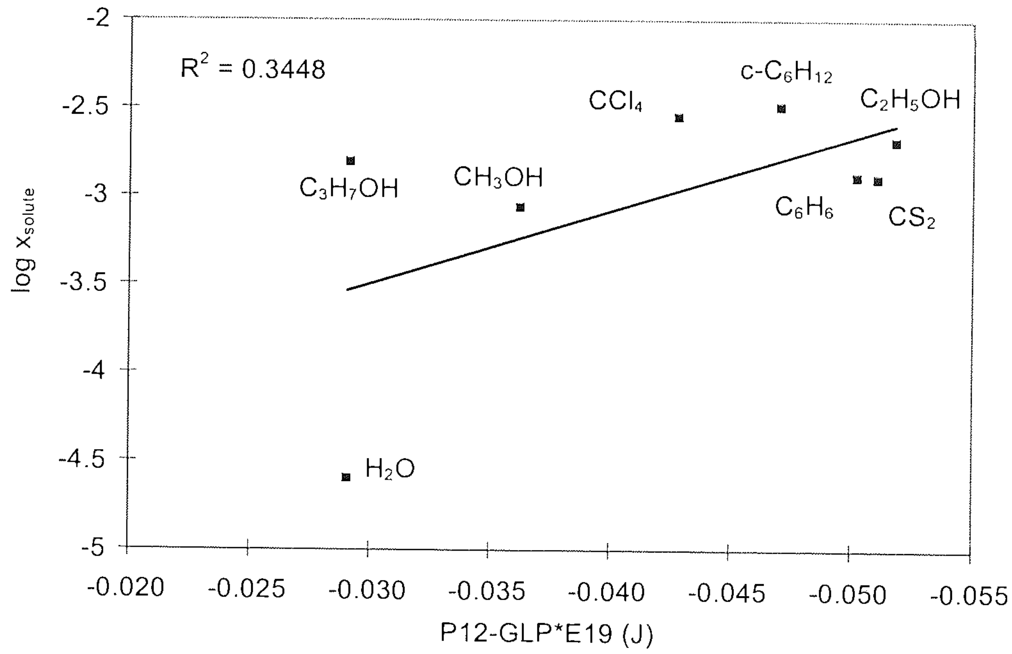

Figure A6.6. Solubilities of **methane** in solvents at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP) calculated by method VDUN.

Appendix 7 - Results of calculations for methane

Table A7-1 shows the results of the calculations for methane using the computer program PP. The first column shows the temperature, the second column displays the calculated values of the heat of vaporization with the equilibrium separation obtained from the heat of vaporization in the third column. The values of the like pair potential obtained from the heat of vaporization option are in column 4. Then follows the molar volume and the equilibrium separation as calculated from the molar volume. Finally, the last column contains the values of the like pair potential obtained from the molar volume option.

T (K)	Hvap (kJ/mol)	R (E-10 m) (Hvap)	PP*E19 (J) (Hvap)	molar volume (cm3/mol)	R (E-10 m) (mol.vol.)	PP*E19 (J) (mol. vol.)
0	11443.43	4.07521	-0.0346	29.6543	4.06035	-0.03553
10	11211.22	4.09084	-0.033585	30.06678	4.07909	-0.034319
20	10970.88	4.10646	-0.0326	30.51191	4.09912	-0.033079
30	10721.62	4.12404	-0.0316	30.99385	4.12059	-0.031811
35	10593.37	4.13283	-0.0311	31.25013	4.13192	-0.031166
40	10462.54	4.1426	-0.0306	31.51754	4.14367	-0.030513
45	10328.98	4.15236	-0.03	31.79687	4.15587	-0.029853
50	10192.54	4.16213	-0.0295	32.08898	4.16856	-0.029185
55	10053.05	4.17287	-0.029	32.39482	4.18176	-0.028509
60	9910.34	4.18361	-0.0284	32.71547	4.19552	-0.027825
65	9764.18	4.19533	-0.0278	33.05212	4.20986	-0.027133
70	9614.37	4.20705	-0.0273	33.40611	4.22483	-0.026433
75	9460.66	4.21975	-0.026668	33.77895	4.24049	-0.025723
80	9302.75	4.23244	-0.0261	34.17235	4.25689	-0.025006
85	9140.34	4.24611	-0.0254	34.58825	4.27409	-0.024279
90	8973.08	4.26076	-0.0248	35.02888	4.29216	-0.023542
95	8800.58	4.27639	-0.0242	35.49681	4.31119	-0.022796
100	8622.37	4.29299	-0.023509	35.995	4.33127	-0.022039
110	8246.7	4.32912	-0.022119	37.09672	4.37501	-0.020494
120	7840.8	4.37014	-0.020659	38.37021	4.42452	-0.0189
130	7397.36	4.41896	-0.019071	39.86792	4.48135	-0.017251
140	6905.68	4.47853	-0.017328	41.66992	4.54788	-0.015536
150	6349.04	4.55373	-0.015395	43.90749	4.62786	-0.013737
160	5698.69	4.65529	-0.013179	46.8188	4.72797	-0.011827
170	4897.14	4.80861	-0.010517	50.91215	4.86192	-0.009746
175	4400.89	4.92678	-0.008897	57.65766	5.06781	-0.007338
180	3791.06	5.11235	-0.006924	58.63636	5.09632	-0.007064
181	3648.14	5.16311	-0.00647	59.71206	5.12729	-0.00678
182	3495.48	5.22268	-0.00599	60.90642	5.16126	-0.006484
184	3152.33	5.38186	-0.0049	62.24967	5.19892	-0.006173
185	2955.24	5.49221	-0.004276	63.78587	5.24134	-0.005845
186	2733.98	5.64064	-0.00359	65.58334	5.29012	-0.005492
187	2478.82	5.86037	-0.00279	67.75742	5.34794	-0.005106
188	2171.52	6.24904	-0.00184	70.53009	5.41991	-0.00467
189	1769.34	7.45314	-0.000598	74.43809	5.51822	-0.004144
189.25	1641.91	8.83498	-0.000206	75.74851	5.55042	-0.003988
189.5	1495.87			77.29631	5.58797	-0.003814
189.75	0			79.20886	5.63368	-0.003514
190				81.77439	5.69386	-0.003369
190.1				83.14144	5.72141	-0.003249
190.2				84.88887	5.76525	-0.003104
190.3				87.43705	5.82237	-0.00291
190.35				89.50606	5.86793	-0.002765
190.39				92.89281	5.94103	-0.002551
190.4				97.82123	6.04429	-0.00228
190.555						0

Table A7-1. The obtained values for equilibrium separations and like pair of potentials calculated as a function of temperature for both the options; the heat of vaporization and molar volume.

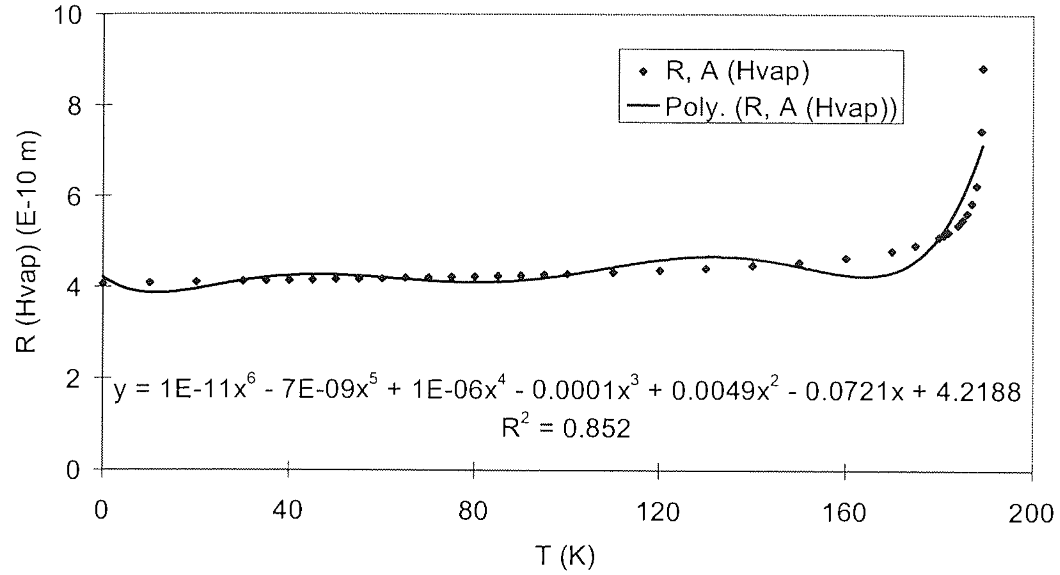

Figure A7.1. Equilibrium separation (calculated from the heat of vaporization) as a function of temperature (up to the critical temperature) and the best fitted curve.

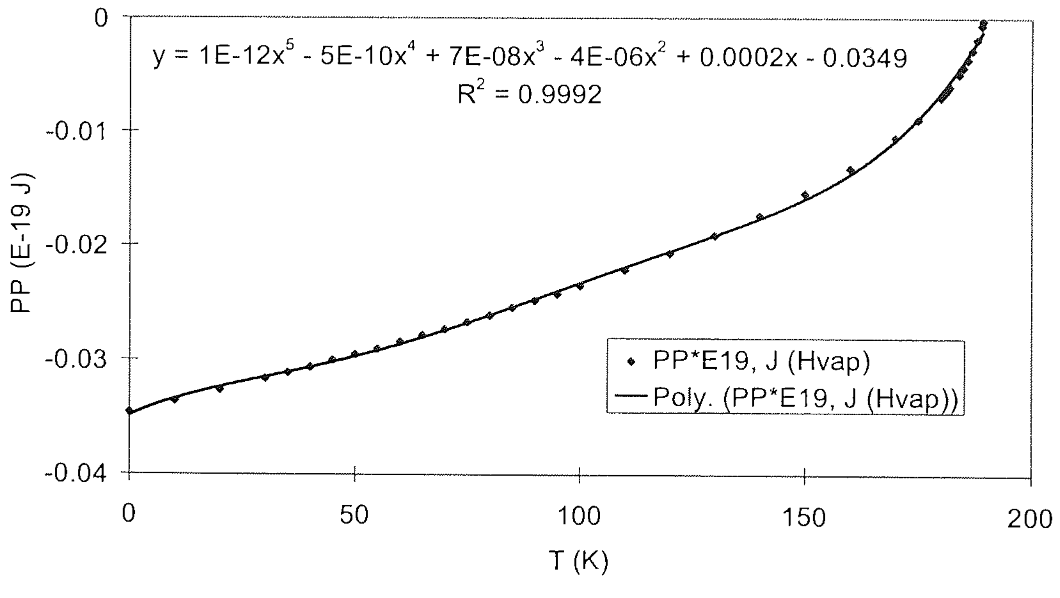

Figure A7.2. The like pair of potentials (calculated from the heat vaporization option) as a function of temperature (up to the critical temperature) and the best fitted curve.

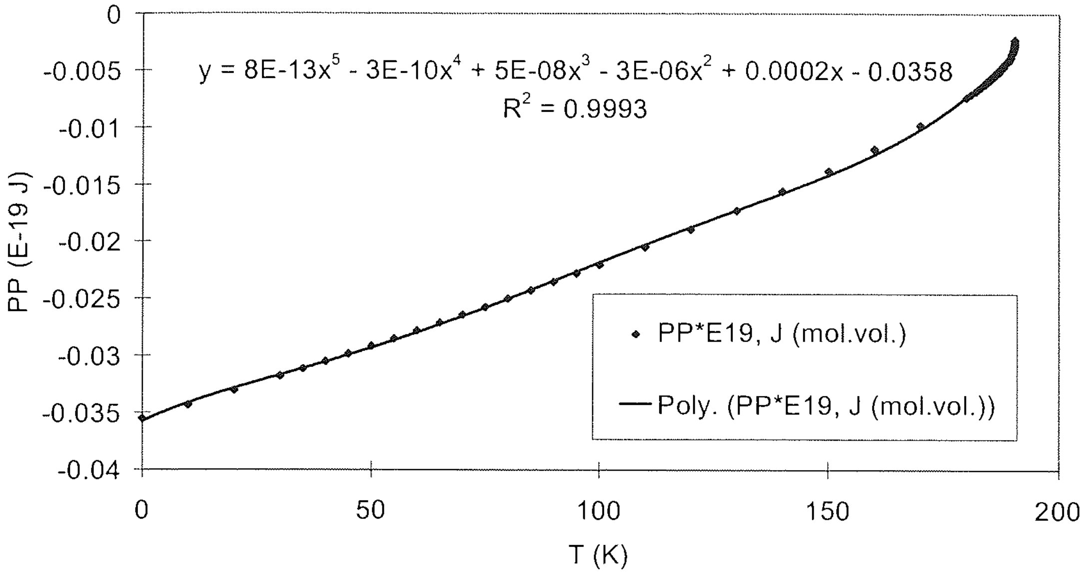

Figure A7.3. The like pair of potentials (calculated from the mol vol heat of vaporization option) as a function of temperature (up to the critical temperature) and the best fitted curve.

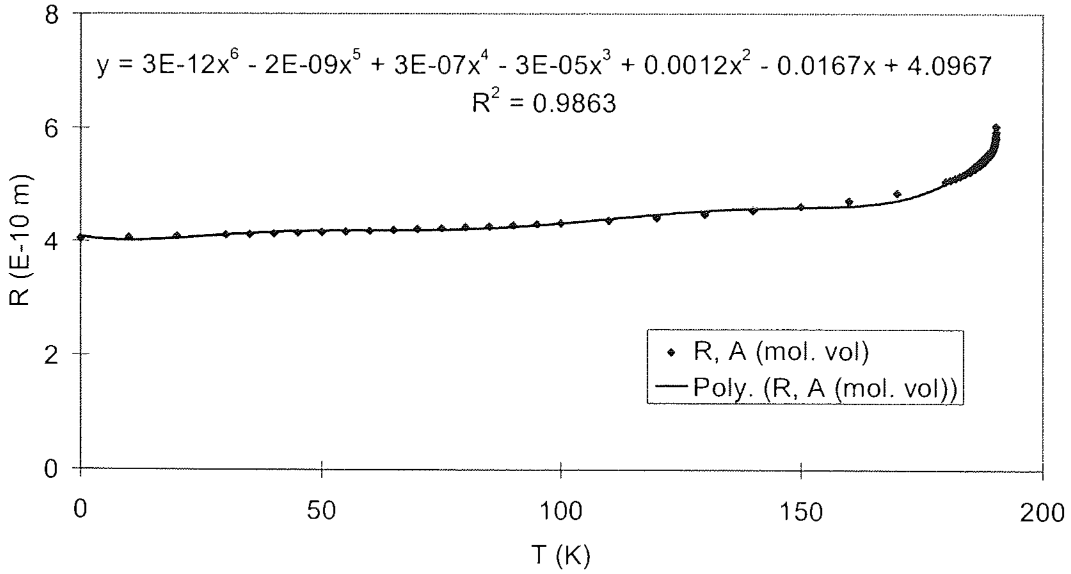

Figure A7.4. Equilibrium separation (calculated from the molar volume option) as a function of temperature (up to the critical temperature) and the best fitted curve.

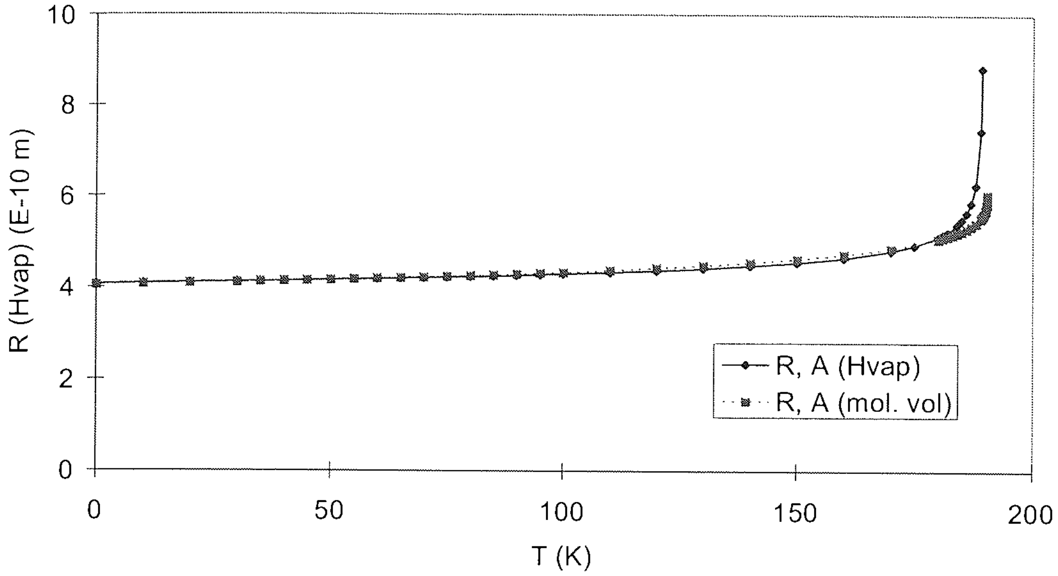

Figure A7.5. The equilibrium separation calculated from both the heat of vaporization and the molar volume options as a function of temperature (up to the critical temperature).

T, K	Hvap, kJ/mol (exp.)
90.68	8720
100	8500
110	8240
111.631	8190
120	7930
130	7560
140	7130
150	6610
160	5960
170	5120
180	3950

Table A7-2. Experimental values of the heat of vaporization as a function of temperature (Perry and Green, 1984).

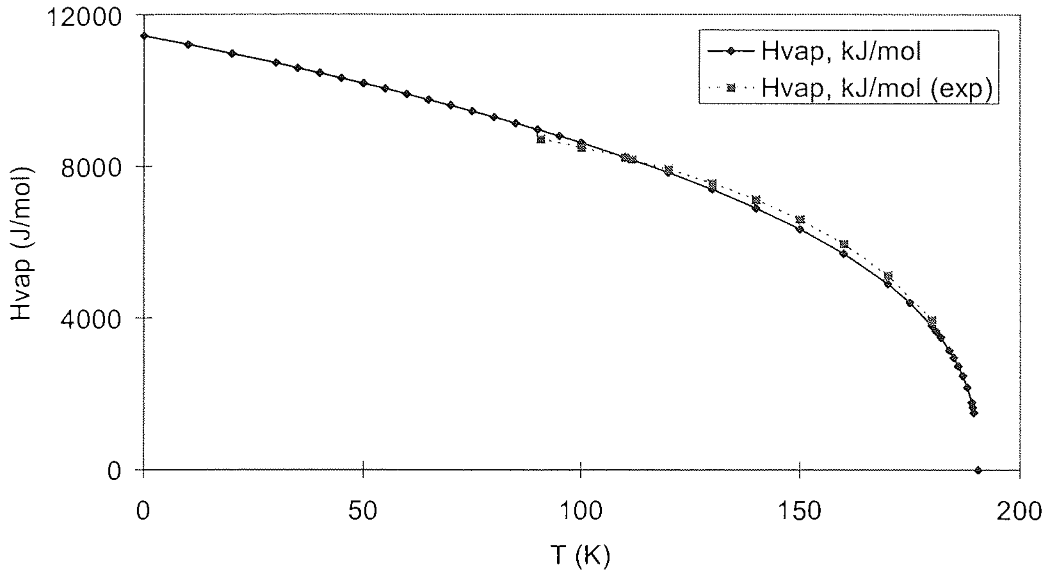

Figure A7.6. The experimental heat of vaporization and the calculated heat of vaporization (Watson's correlation) as a function of temperature.

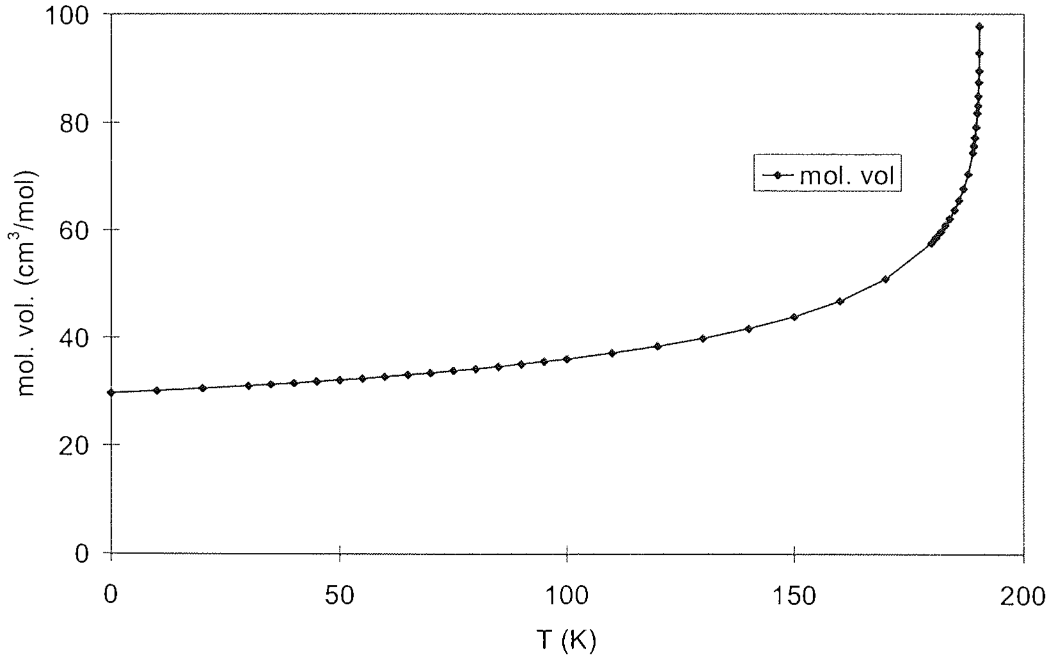

Figure A7.7. The molar volume as a function of temperature.

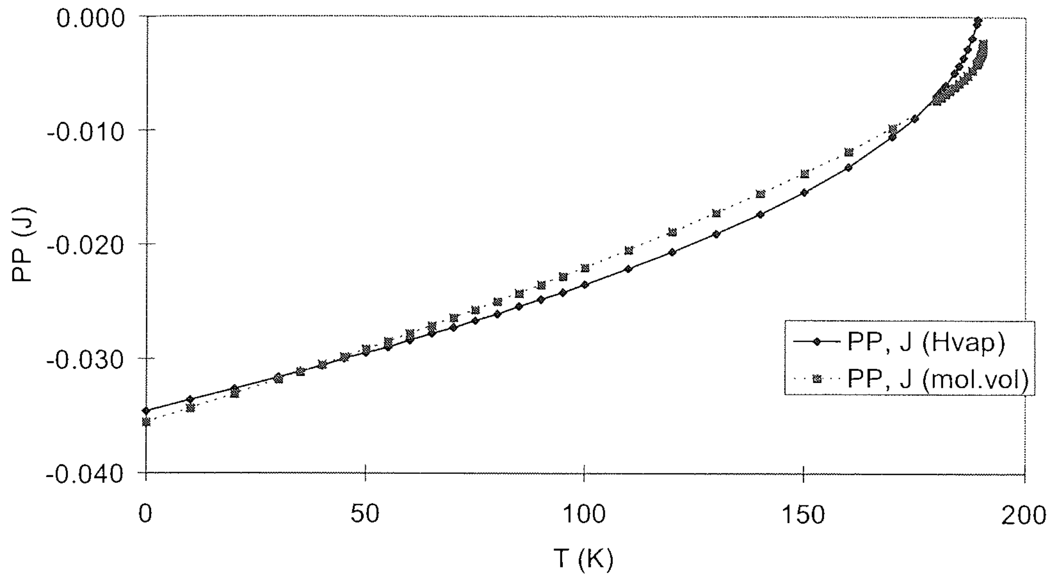

Figure A7.8. The like pair of potentials calculated from both the heat of vaporization and the molar volume options as a function of temperature (up to the critical temperature).

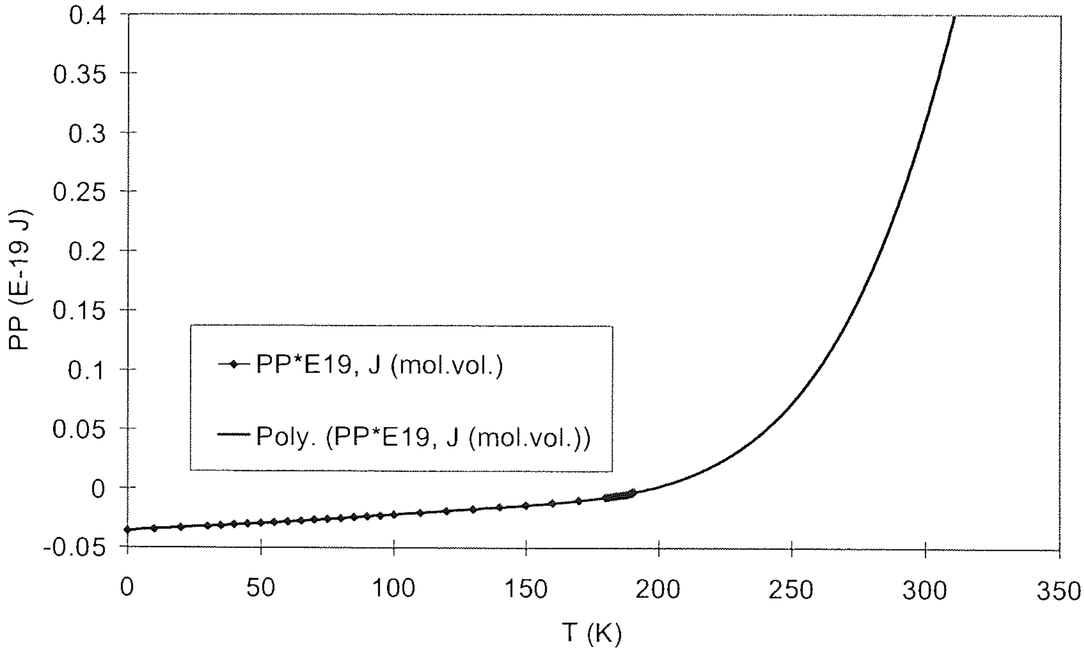

Figure A7.9. The like pair of potentials (calculated from the molar volume option) as a function of temperature (extrapolated up to 350 K) and the best fitted curve.

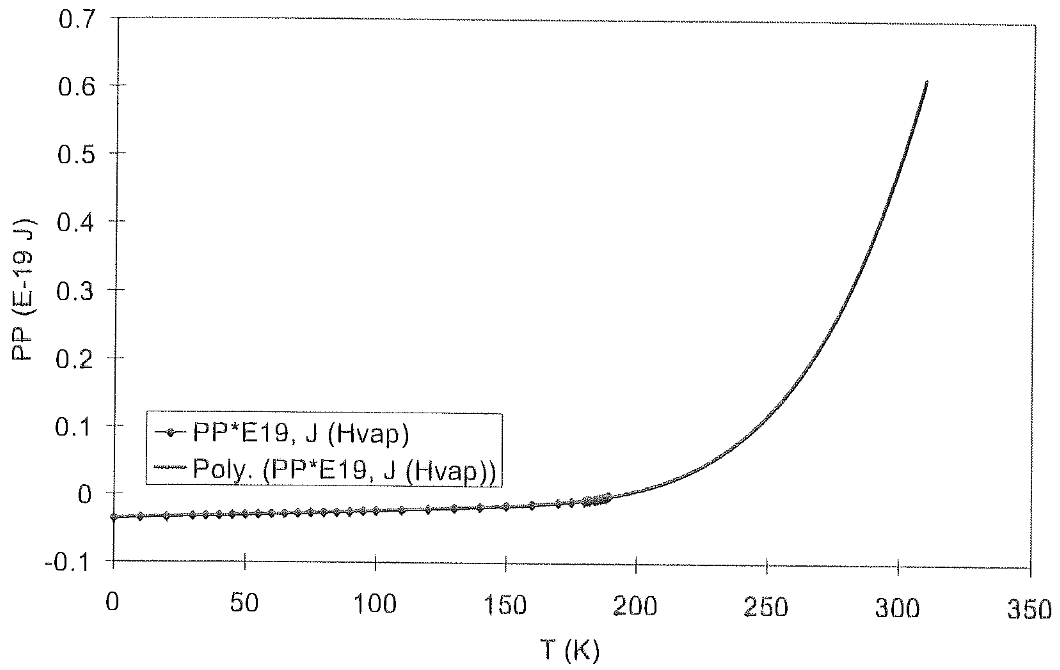

Figure A7.10. The like pair of potentials (calculated from the heat of vaporization) as a function of temperature (extrapolated up to 350 K) and the best fitted curve.

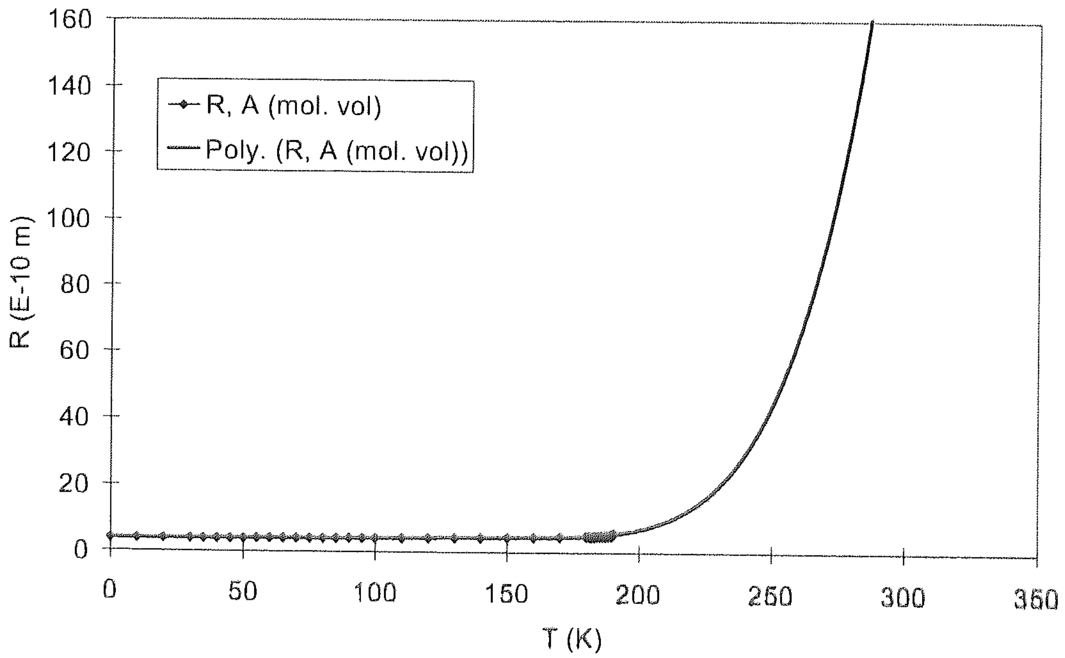

Figure A7.11. Equilibrium separation (calculated from the molar volume option) as a function of temperature (extrapolated up to 350 K) and the best fitted curve.

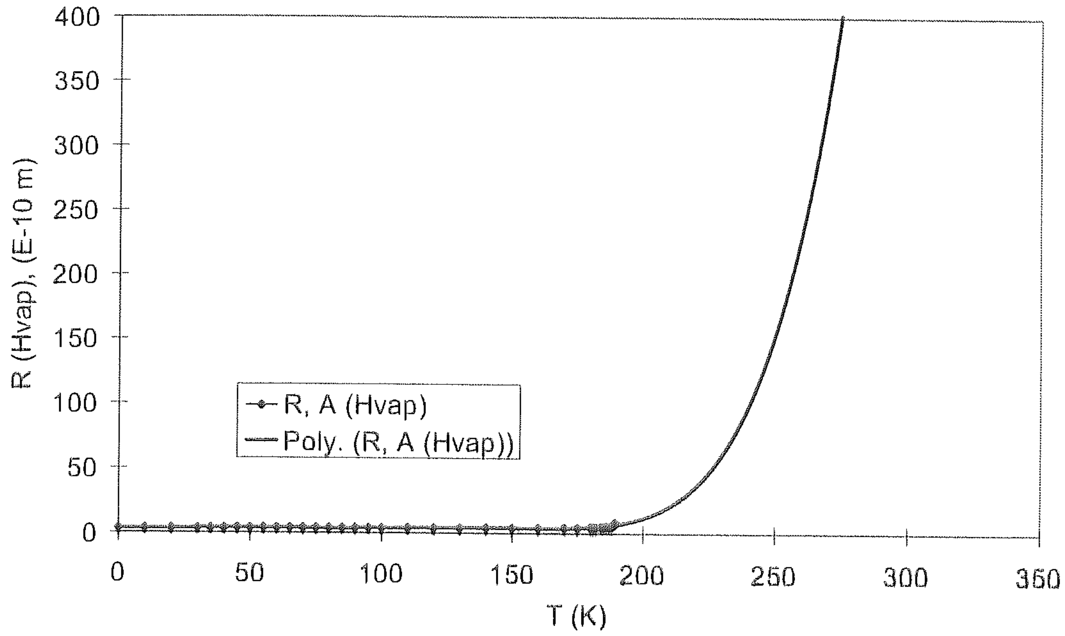

Figure A7.12. Equilibrium separation (calculated from the heat of vaporization option) as a function of temperature (extrapolated up to 350 K) and the best fitted curve.

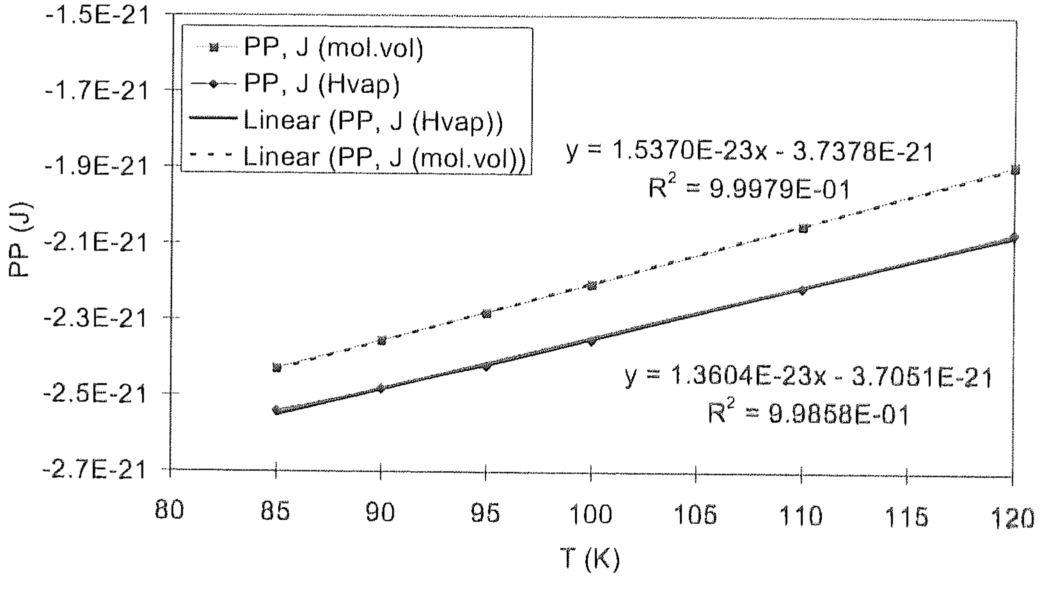

Figure A7.13. The like pair of potentials as a function of temperature in the interval: the triple point to the boiling point and the best fitting curves.

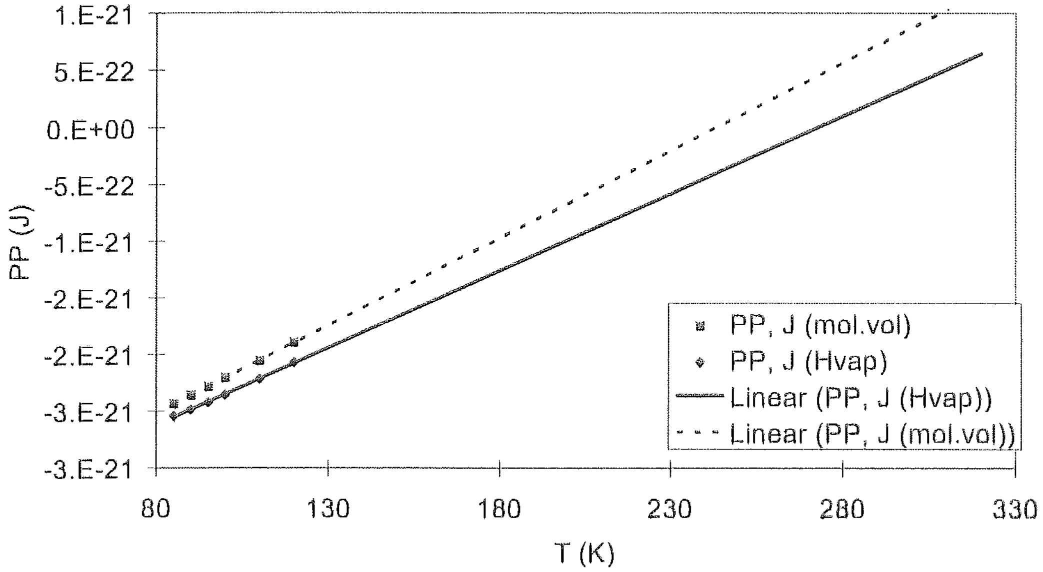

Figure A7.14. The like pair of potentials as a function of temperature and the best fitting curves extrapolated to 350 K.

Appendix 8 - Results of the extrapolating method

T (K)	R (mol.vol.) (10^{-10}m)	R (Hvap) (10^{-10}m)
100	4.57678	4.63852
104	4.58674	4.64438
110	4.60206	4.65317
120	4.62872	4.66977
130	4.65692	4.68735
140	4.68686	4.70591
150	4.71875	4.72739
160	4.75288	4.74888
169.3	4.78693	4.77231
170	4.7896	4.77427
180	4.82933	4.80161

Table A8-1. Values of the equilibrium separation as a function of temperature calculated from the molar volume or the heat of vaporization option for **ethylene**.

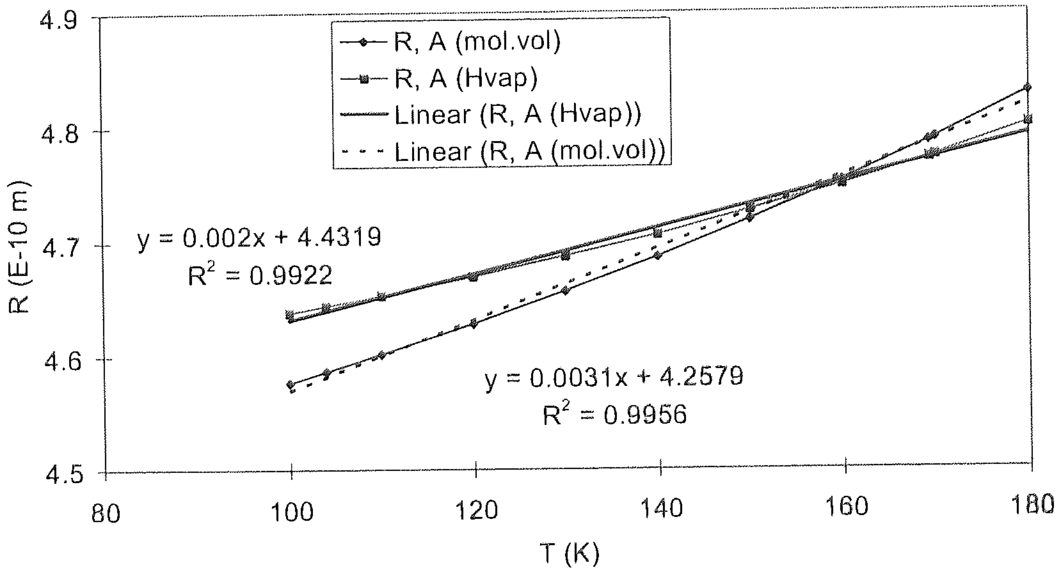

Figure A8.1 Equilibrium separation calculated from both the molar volume and the heat of vaporization as a function of temperature in the interval from the triple point to the boiling point and the best linear fitted curves for **ethylene**.

T (K)	R (mol.vol.) (10^{-10}m)	R (Hvap) (10^{-10}m)
24.5	3.32735	3.02977
24.75	3.32957	3.0327
25	3.33185	3.03562
25.25	3.33419	3.03953
25.5	3.3366	3.04344
25.75	3.33907	3.04637
26	3.34161	3.05027
26.25	3.34422	3.05369
26.5	3.3469	3.05711
26.75	3.34965	3.06102
27	3.35247	3.06492
27.1	3.35363	3.06687

Table A8-2. Values of the equilibrium separation as a function of temperature calculated from the molar volume or the heat of vaporization option for **neon**.

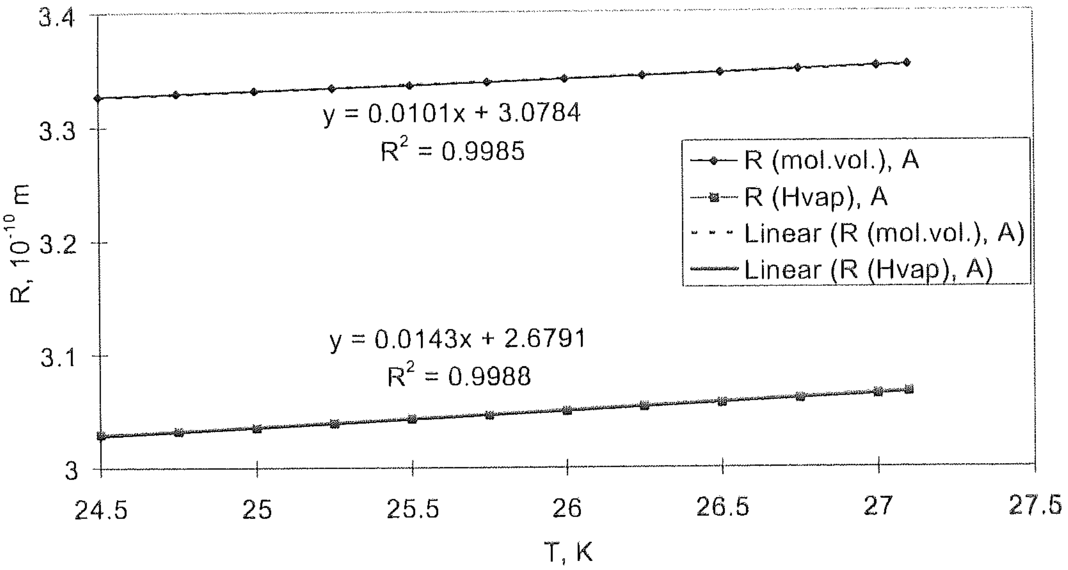

Figure A8.2. Equilibrium separation calculated from both the molar volume and the heat of vaporization as a function of temperature in the interval from the triple point to the boiling point and the best linear fitted curves for **neon**.

T (K)	R (mol.vol.) $(10^{-10}m)$	R (Hvap) $(10^{-10}m)$
70	3.93285	3.70019
80	3.97613	3.74316
83.8	3.99434	3.76074
85	4.00032	3.7666
87.28	4.01201	3.77832
90	4.02654	3.79199
95	4.05509	3.82031

Table A8-3. Values of the equilibrium separation as a function of temperature calculated from the molar volume or the heat of vaporization option for **argon**.

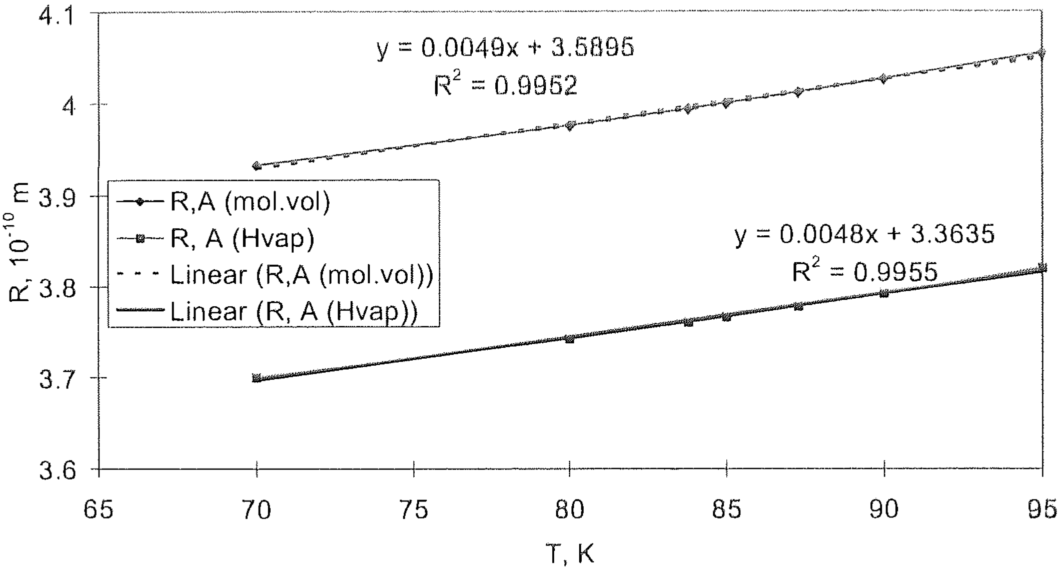

Figure A8.3. Equilibrium separation calculated from both the molar volume and the heat of vaporization as a function of temperature in the interval from the triple point to the boiling point and the best linear fitted curves for **argon**.

T (K)	R (mol.vol.) (10^{-10}m)	R (Hvap) (10^{-10}m)
60	4.22199	3.90575
65	4.24503	3.92723
68.1	4.2604	3.94188
70	4.27026	3.95164
80	4.32866	4.00633
81.7	4.33984	4.0161
85	4.36276	4.03758
90	4.40096	4.07372

Table A8-4. Values of the equilibrium separation as a function of temperature calculated from the molar volume or the heat of vaporization option for **carbon monoxide**.

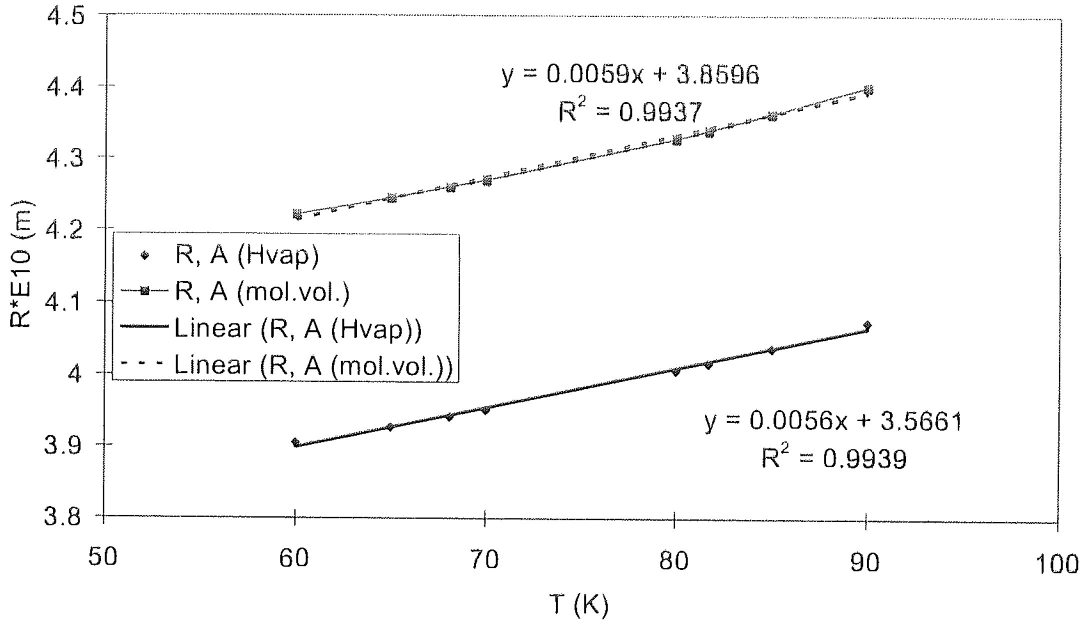

Figure A8.4. Equilibrium separation calculated from both the molar volume and the heat of vaporization as a function of temperature in the interval from the triple point to the boiling point and the best linear fitted curves for **carbon monoxide**.

T (K)	R (mol.vol.) (10^{-10}m)	R (Hvap) (10^{-10}m)
9	3.75244	3.85612
10	3.75744	3.87174
11	3.76333	3.88835
12	3.77019	3.90592
13	3.77807	3.9235
14	3.78706	3.94303
15	3.79725	3.96354
16	3.80876	3.98502
17	3.8217	4.00846
18	3.83624	4.03385
19	3.85256	4.06022
20	3.87087	4.08952
20.3	3.87679	4.09928
21	3.89145	4.12174
22	3.91461	4.15788
23	3.94079	4.19694
24	3.97052	4.24186

Table A8-5. Values of the equilibrium separation as a function of temperature calculated from the molar volume or the heat of vaporization option for **hydrogen**.

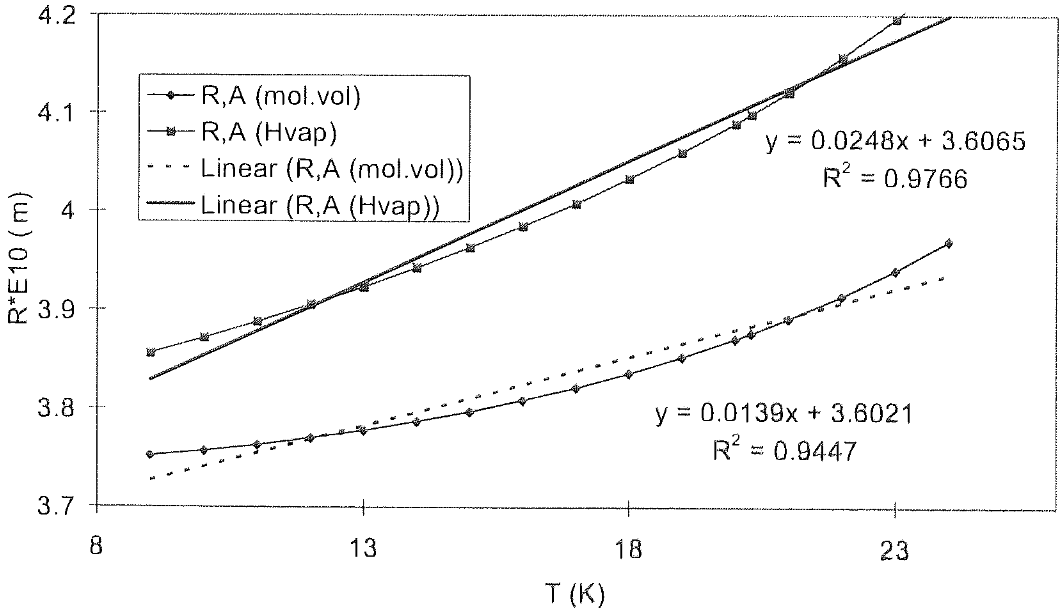

Figure A8.5. Equilibrium separation calculated from both the molar volume and the heat of vaporization as a function of temperature in the interval from the triple point to the boiling point and the best linear fitted curves for **hydrogen**.

T (K)	R (mol.vol.) (10^{-10}m)	R (Hvap) (10^{-10}m)
60	4.17941	3.88922
63.148	4.19658	3.90386
65	4.20711	3.91363
70	4.23732	3.94097
75	4.27046	3.97125
77.347	4.28717	3.9859
80	4.30707	4.00445
85	4.34786	4.04254

Table A8-6. Values of the equilibrium separation as a function of temperature calculated from the molar volume or the heat of vaporization option for **nitrogen**.

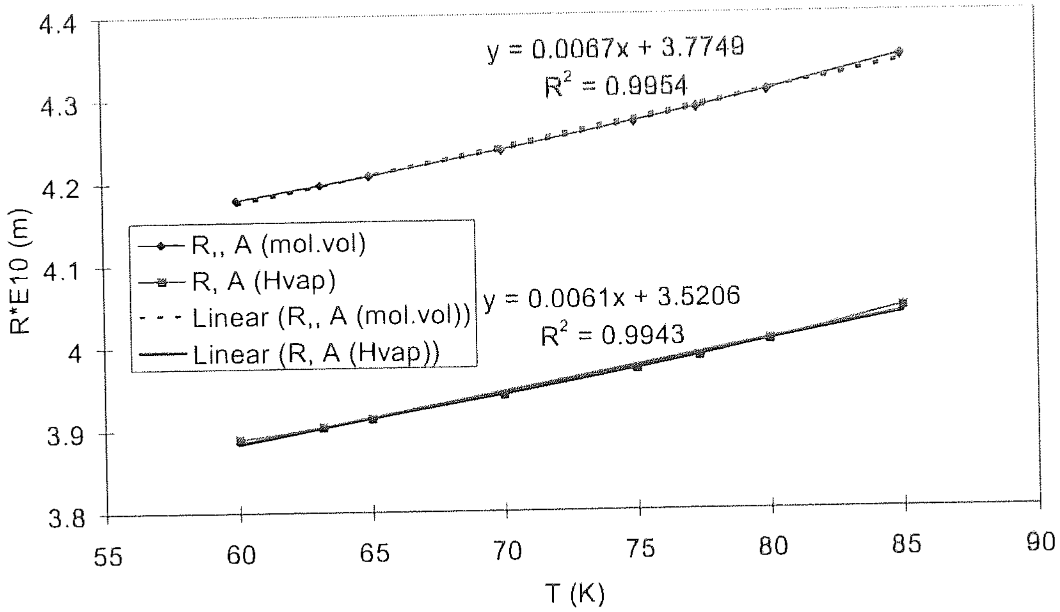

Figure A8.6. Equilibrium separation calculated from both the molar volume and the heat of vaporization as a function of temperature in the interval from the triple point to the boiling point and the best linear fitted curves for **nitrogen**.

T (K)	R (mol.vol.) (10^{-10}m)	R (Hvap) (10^{-10}m)
50	3.81596	3.52716
54.4	3.8303	3.53888
60	3.84957	3.55451
70	3.8872	3.58576
80	3.92976	3.62091
90	3.97856	3.6629
90.2	3.97961	3.66388
95	4.00585	3.68634
100	4.03547	3.71173

Table A8-7. Values of the equilibrium separation as a function of temperature calculated from the molar volume or the heat of vaporization option for **oxygen**.

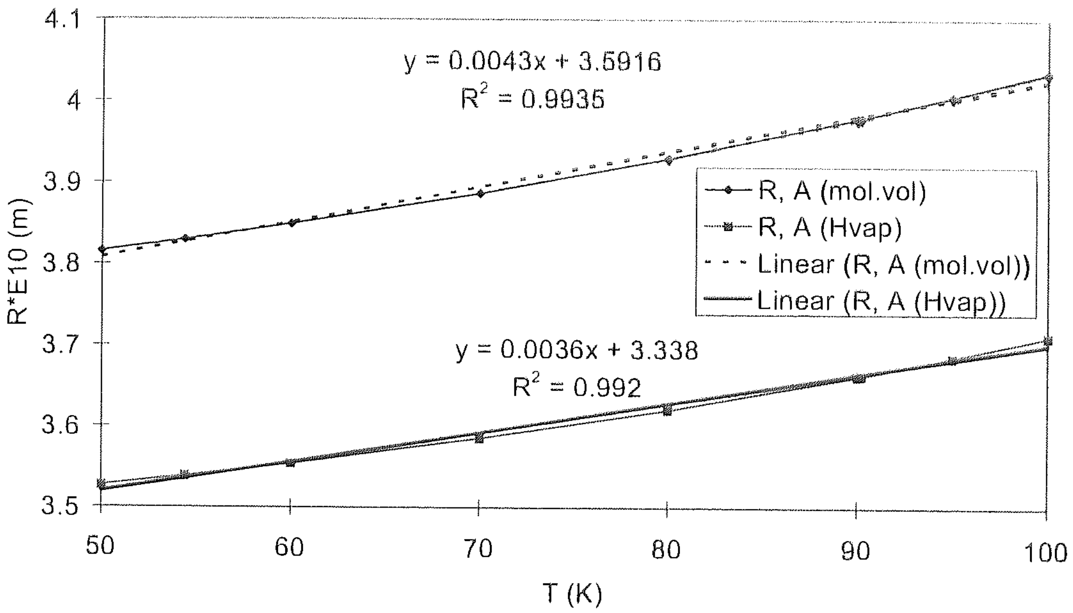

Figure A8.7. Equilibrium separation calculated from both the molar volume and the heat of vaporization as a function of temperature in the interval from the triple point to the boiling point and the best linear fitted curves for **oxygen**.

Appendix 9 - Results of the VDUD calculation method

A9.1 Results of VDUD calculations for a series of solutes dissolved in a single solvent

All tables in this Appendix show the mixture in the first column, then the experimental solubility at 298.15 K and partial pressure of the solute of 101.325 kPa (from Table A3-1), the next column displays the base 10 logarithm of the solubility, then follows the unlike London pair potential for the mixture. For some solvents, an other column showing the unlike geometric pair potential follows. In some cases, the geometric mean pair potentials have been calculated and are shown in the table, but not plotted in a graph.

The experimental solubility data are from Fogg and Gerard (1991) or IUPAC Solubility Data Series (Clever, 1979 (vol. 1), Clever, 1980 (vol. 4), Young, 1981 (vol. 5/6), Battino, 1981 (vol. 7), Hayduk, 1982 (vol. 9), Battino, 1982 (vol. 10), Hayduk, 1986 (vol. 24), and Clever and Young, 1987 (vol. 27/28)).

The points on the graphs represent the pair potential, the line is the best fitted straight line through the points and the R^2 is the line correlation coefficient.

A9.1.1 Results of molar volume calculations

VDUD solvent-solute	x_{solute}	log x_{solute}	**P12- GLP*E19 (J)**	**P12- GM*E19 (J)**
C_6H_6-CH_4	0.00209	-2.679853714	-2.257200E-02	-2.811700E-02
C_6H_6-CO_2	0.00912	-2.040005162	-2.426800E-02	-3.045100E-02
C_6H_6-Ar	0.000882	-3.054531415	-1.210000E-02	-1.965000E-02
C_6H_6-N_2	0.000445	-3.351639989	-9.336000E-03	-1.378600E-02
C_6H_6-C_2H_6	0.0149	-1.826813732	-2.712500E-02	-3.255900E-02
C_6H_6-C_2H_4	0.01185	-1.92628165	-4.295800E-02	-4.844500E-02
C_6H_6-H_2	0.000259	-3.586532587	-1.282000E-03	-2.324000E-03
C_6H_6-O_2	0.00081	-3.091514981	-1.403200E-02	-1.904700E-02
C_6H_6-CO	0.00065	-3.187086643	-1.082800E-02	-1.563400E-02
C_6H_6-n-C_3H_8	0.0573	-1.241845378	-5.6392E-02	-6.074915E-02

VDUD solvent-solute	x_{solute}	log x_{solute}	**P12- GLP*E-19 (J)**	**P12- GM*E-19 (J)**
CCl_4-CO_2	0.01	-2	-2.217700E-02	-2.381700E-02
CCl_4-CH_4	0.002856	-2.544241797	-2.065800E-02	-2.199200E-02
CCl_4-Ar	0.00135	-2.869666232	-1.173800E-02	-1.536500E-02
CCl_4-N_2	0.000641	-3.19314197	-9.053000E-03	-1.078300E-02
CCl_4-H_2	0.000323	-3.491470281	-1.311000E-03	-1.818000E-03
CCl_4-O_2	0.0012	-2.920818754	-1.316700E-02	-1.489700E-02
CCl_4-CO	0.000865	-3.062983893	-1.047900E-02	-1.222800E-02
CCl_4-C_2H_4	0.0148	-1.829738285	-3.704900E-02	-3.791220E-02
CCl_4-C_2H_6	0.0211	-1.675717545	-2.479700E-02	-2.546500E-02
CCl_4-n-C_3H_8	0.0813	-1.089909454	-4.7485E-02	-4.751354E-02
CCl_4-n-C_4H_{10}	0.339	-0.469800302	-6.5446E-02	-6.68428E-02

VDUD solvent-solute	x_{solute}	log x_{solute}	**P12 - GLP*E19 (J)**	**P12- GM*E19 (J)**
c-C_6H_{12}-CH4	0.00327	-2.485452247	-2.161300E-02	-2.507700E-02
c-C_6H_{12}-Ar	0.00114	-2.943095149	-1.155300E-02	-1.752100E-02
c-C_6H_{12}-H_2	0.000414	-3.382999659	-1.294000E-03	-2.081700E-03
c-C_6H_{12}-N_2	0.000768	-3.11463878	-9.061000E-03	-1.229550E-02
c-C_6H_{12}-O_2	0.00123	-2.910094889	-1.343500E-02	-1.698700E-02
c-C_6H_{12}-CO	0.000999	-3.000434512	-1.054500E-02	-1.395040E-02
c-C_6H_{12}-C_2H_6	0.0233	-1.632644079	-2.630800E-02	-2.903880E-02
c-C_6H_{12}-CO_2	0.00759	-2.119758224	-2.311700E-02	-2.715840E-02
c-C_6H_{12} - n-C_3H_8	0.091	-1.040958608	-5.2912E-02	-5.4181-02

VDUD solvent-solute	x_{solute}	log x_{solute}	**P12 - GLP*E19 (J)**
$CHCl_3$-Ar	0.000592	-3.227678293	-1.008500E-02
$CHCl_3$ -H_2	0.00022	-3.657577319	-1.116000E-03
$CHCl_3$ -N_2	0.000445	-3.351639989	-7.739000E-03
$CHCl_3$ -CO	0.000665	-3.177178355	-8.959000E-03
$CHCl_3$-CO_2	0.0128	-1.89279003	-1.888600E-02

Table A9-1. The obtained unlike pair potentials calculated by method VDUD and the experimental solubility (x_{solute}) for gases in liquids at 298.15 K, 101.325 kPa (continued over).

VDUD solvent-solute	x_{solute}	log x_{solute}	P12 - GLP*E19 (J)
CS_2 -CH_4	0.001309	-2.883060353	-2.339200E-02
CS_2 -Ar	0.000486	-3.31309573	-1.384000E-02
CS_2 -H_2	0.000159	-3.797784224	-1.418000E-03
CS_2 -N_2	0.000222	-3.654626269	-1.028000E-02
CS_2 -O_2	0.000439	-3.35753548	-1.519200E-02
CS_2 -CO	0.00036	-3.443697499	-1.187700E-02
CS_2 -C_2H_6	0.0107	-1.970616222	-2.713300E-02
CS_2 -CO_2	0.00328	-2.484126156	-2.525200E-02
CS_2 -n-C_3H_8	0.0446	-1.350665141	-5.2065E-02

VDUD solvent-solute	x_{solute}	log x_{solute}	P12 - GLP*E19 (J)	P12- GM*E19 (J)
H_2O-CH_4	0.00002548	-4.593800576	-1.203300E-02	-1.393400E-02
H_2O-Ar	0.00002519	-4.598771833	-7.399000E-03	-9.735000E-03
H_2O-H_2	0.00001411	-4.850472986	-5.980000E-04	-1.137000E-03
H_2O-N_2	0.00001183	-4.927015255	-4.993000E-03	-6.832000E-03
H_2O-O_2	0.00002293	-4.639595945	-8.024000E-03	-9.439000E-03
H_2O-CO	0.0000172	-4.764471553	-5.847000E-03	-7.750000E-03
H_2O-C_2H_4	0.00008582	-4.06641149	-2.154300E-02	-1.509030E-02
H_2O-C_2H_6	0.000034	-4.468521083	-1.270500E-02	-2.402200E-02
H_2O-CO_2	0.0006116	-3.213532523	-1.288200E-02	-1.613500E-02
H_2O-n-C_3H_8	0.00002732	-4.563519305	-2.4876E-02	-3.0105E-02
H_2O-n-C_4H_{10}	0.00002244	-4.648977147	-3.438E-02	-4.23533-02

VDUD solvent-solute	x_{solute}	log x_{solute}	P12-GLP*E19 (J)	P12-GM*E19 (J)
CH_3OH-CH_4	0.000871	-3.059981845	-0.01554	-0.01738598
CH_3OH-Ar	0.000447	-3.349692477	-0.008755	-0.012147506
CH_3OH-H_2	0.000161	-3.793174124	-0.00082	-0.001443262
CH_3OH-N_2	0.000276	-3.559090918	-0.006383	-0.008524578
CH_3OH-O_2	0.000415	-3.381951903	-0.009973	-0.011777484
CH_3OH-CO	0.000327	-3.485452247	-0.007472	-0.009671909
CH_3OH-C_2H_4	0.0047	-2.327902142	-0.028618	-0.029973157
CH_3OH-C_2H_6	0.00393	-2.40560745	-0.017595	-0.020132899
CH_3OH-Ne	0.0000804	-4.094743951	-0.001306	-0.001921613
CH_3OH-n-C_3H_8	0.0115	-1.93930216	-0.035302	-0.03756389
CH_3OH-n-C_4H_{10}	0.0398	-1.400116928	-0.050071	-0.052845488
CH_3OH-CO_2	0.00639	-2.194499142	-0.016616	-0.018829146

Table A9-1. The obtained unlike pair potentials calculated by method VDUD and the experimental solubility (x_{solute}) for gases in liquids at 298.15 K, 101.325 kPa (continued over).

VDUD solvent-solute	x_{solute}	log x_{solute}	P12-GLP*E19 (J)	P12-GM*E19 (J)
C_2H_5OH-CH_4	0.00128	-2.89279003	-0.020601	-0.02909222
C_2H_5OH-Ar	0.0006257	-3.203633845	-0.01068	-0.020326604
C_2H_5OH-N_2	0.000357	-3.447331784	-0.008036	-0.014264305
C_2H_5OH-O_2	0.0005825	-3.23470407	-0.012701	-0.019707441
C_2H_5OH-CO	0.000449	-3.347753659	-0.009449	-0.01618415
C_2H_5OH-C_2H_6	0.00666	-2.176525771	-0.024015	-0.033688683
C_2H_5OH-Ne	0.000109	-3.962573502	-0.001615	-0.003215465
C_2H_5OH-H_2	0.000206	-3.68613278	-0.001042	-0.002415031
C_2H_5OH-n-C_3H_8	0.0228	-1.642065153	-0.051803	-0.062856221
C_2H_5OH-n-C_4H_{10}	0.0815	-1.088842391	-0.079148	-0.088427148
C_2H_5OH-CO_2	0.00689	-2.161780778	-0.021915	-0.031507093

VDUD solvent-solute	x_{solute}	log x_{solute}	P12-GLP*E19 (J)	P12-GM*E19 (J)
C_3H_7OH-CH_4	0.00156	-2.806875402	-0.025621	-0.036148436
C_3H_7OH-Ar	0.000777	-3.109578981	-0.012092	-0.02525675
C_3H_7OH-H_2	0.000231	-3.63638802	-0.001212	-0.003000789
C_3H_7OH-N_2	0.000402	-3.395773947	-0.009369	-0.017729834
C_3H_7OH-O_2	0.000503	-3.298432015	-0.015141	-0.024487411
C_3H_7OH-CO	0.0005193	-3.284581677	-0.011099	-0.020109558
C_3H_7OH-CO_2	0.00772	-2.1123827	-0.027072	-0.03914874

Table A9-1. The obtained unlike pair potentials calculated by method VDUD and the experimental solubility (x_{solute}) for gases in liquids at 298.15 K, 101.325 kPa.

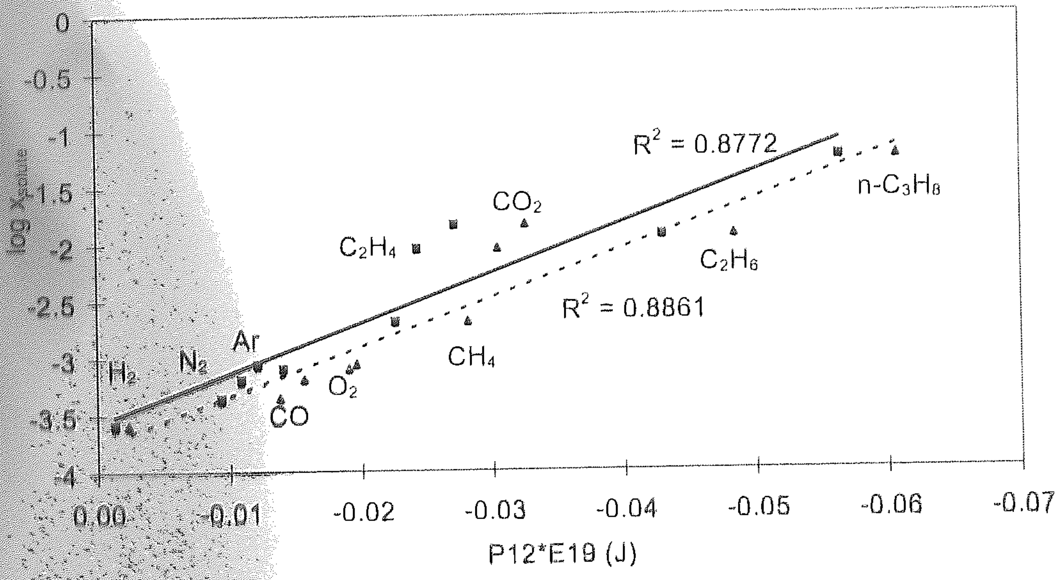

Figure A9.1. Solubilities of gases in **benzene** at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP, ■ points and – line) and the geometric mean unlike pair potential (P12-GM, ▲ points and -- line) calculated by method VDUD.

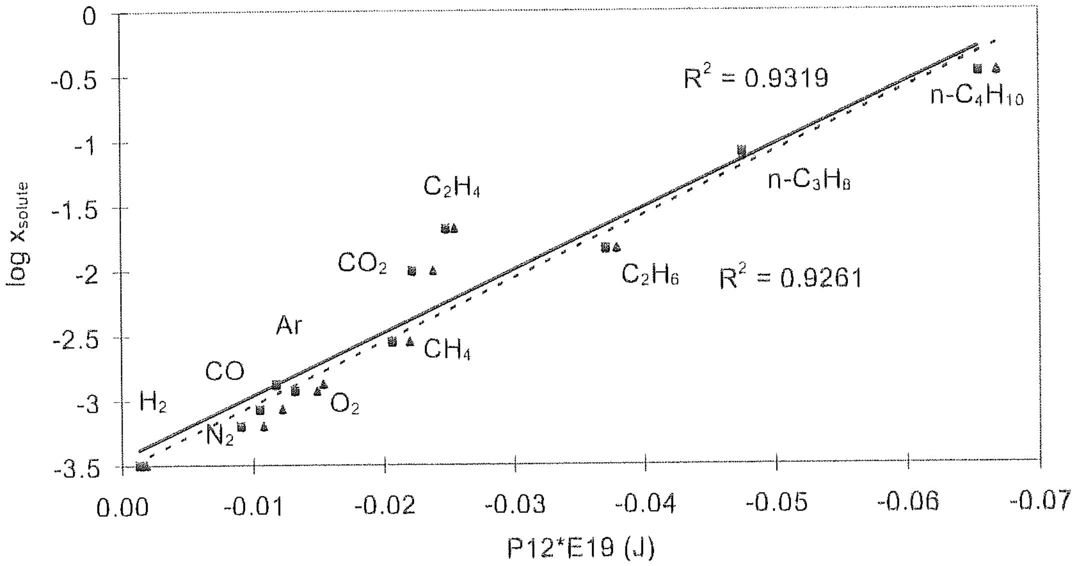

Figure A9.2. Solubilities of gases in **carbon tetrachloride** at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP, ■ points and – line) and the geometric mean unlike pair potential (P12-GM, ▲ points and -- line) calculated by method VDUD.

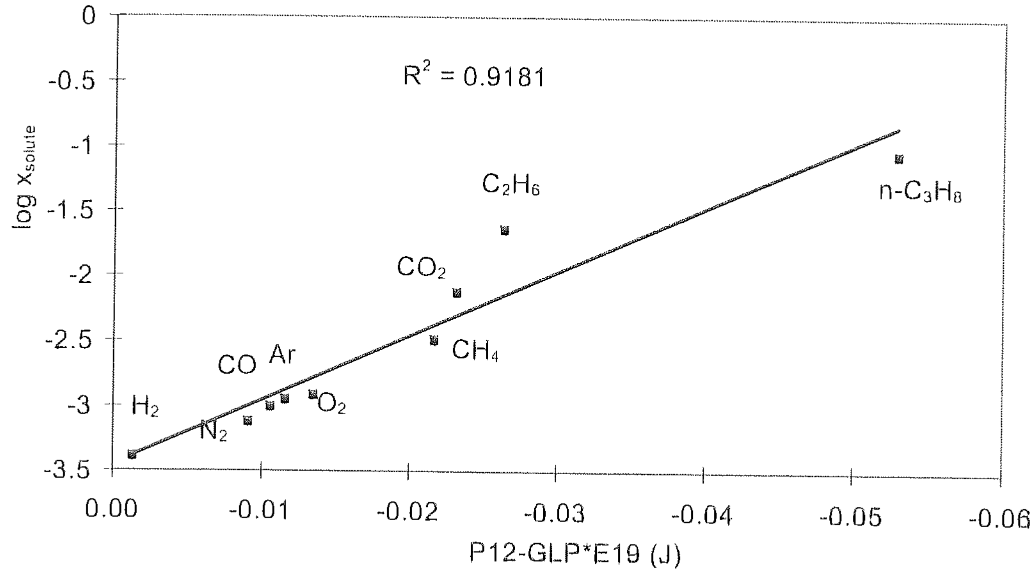

Figure A9.3. Solubilities of gases in ***cyclo* hexane** at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP) calculated by method VDUD.

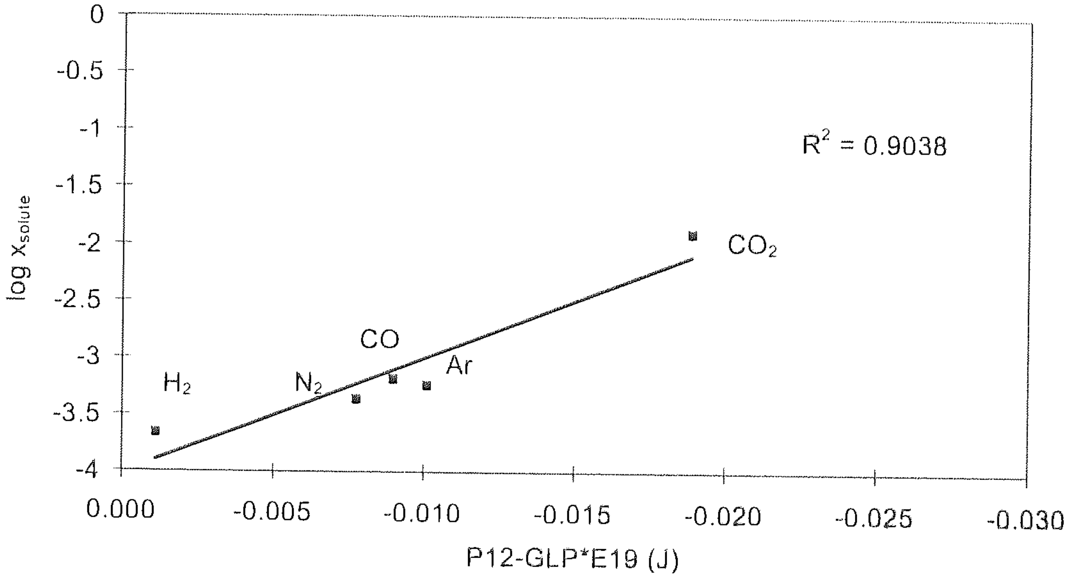

Figure A9.4. Solubilities of gases in **chloroform** at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP) calculated by method VDUD.

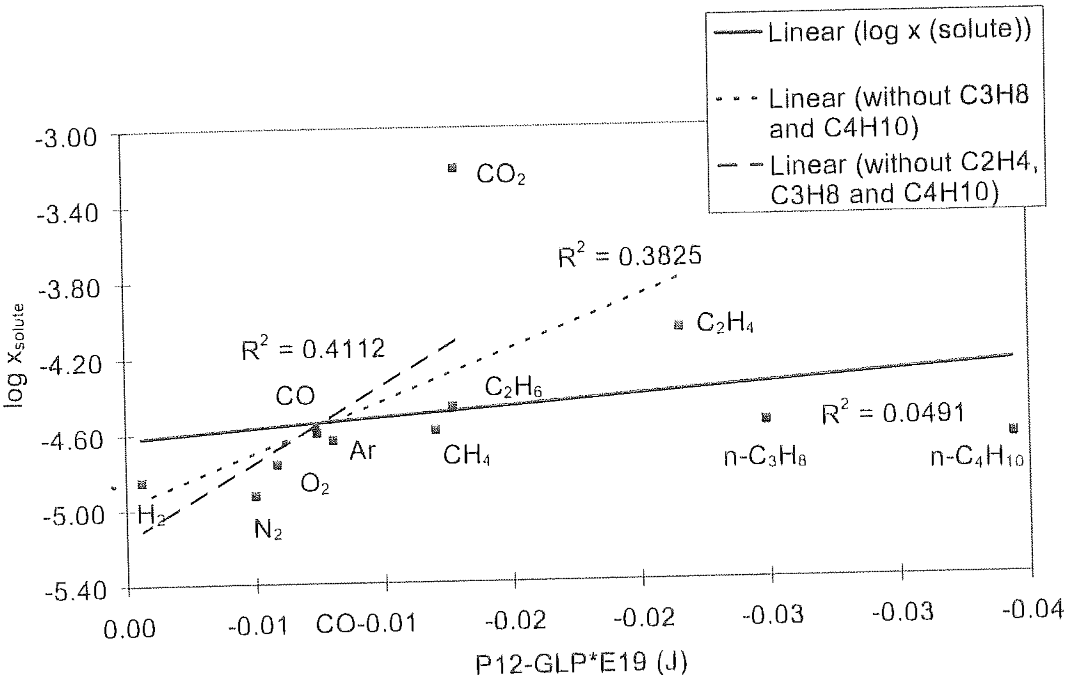

Figure A9.5. Solubilities of gases in **water** at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP) calculated by method VDUD. The continuous line (——) is the trendline though all the points, the dashed line (- -) is the trendline though the points excluding the datapoints for propane and n-butane, while the second dashed line (— —) is the trendline though the points excluding the datapoints for propane, n-butane, and ethylene.

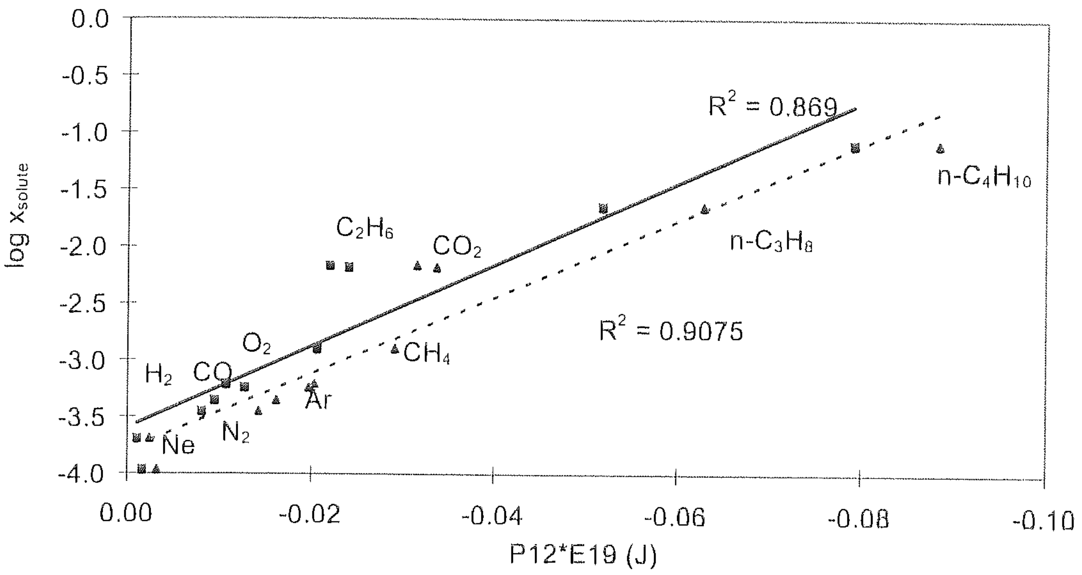

Figure A9.6. Solubilities of gases in **ethanol** at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP, ■ points and — line) and the geometric mean unlike pair potential (P12-GM, ▲ points and -- line) calculated by method VDUD.

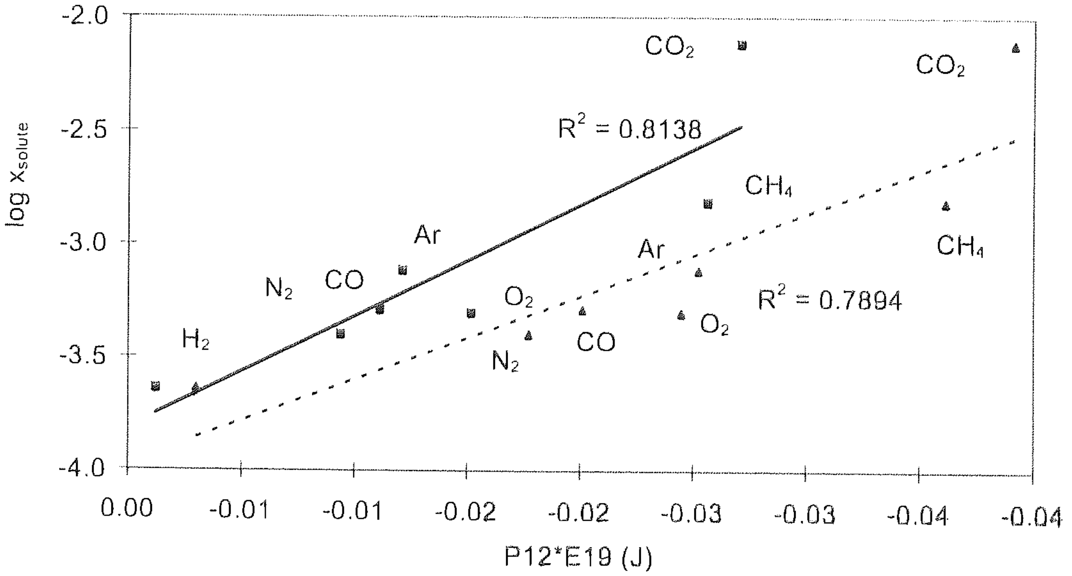

Figure A9.7. Solubilities of gases in **1-propanol** at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP, ■ points and – line) and the geometric mean unlike pair potential (P12-GM, ▲ points and -- line) calculated by method VDUD.

A9.1.2 Interchange energy

VDUD solvent-solute	x_{solute}	log x_{solute}	P11*E19 (J)	P22*E19 (J)	P12-GLP*E19 (J)	w′ (GLP)*E19 (J)
C_2H_5OH-CH_4	0.00128	-2.89279003	-0.006385	-0.132554	-0.020601	0.0488685
C_2H_5OH -Ar	0.0006257	-3.203633845	-0.003117	-0.132554	-0.01068	0.0571555
C_2H_5OH -N_2	0.000357	-3.447331784	-0.001535	-0.132554	-0.008036	0.0590085
C_2H_5OH- O_2	0.0005825	-3.23470407	-0.00293	-0.132554	-0.012701	0.055041
C_2H_5OH -CO	0.000449	-3.347753659	-0.001976	-0.132554	-0.009449	0.057816
C_2H_5OH - C_2H_6	0.00666	-2.176525771	-0.008562	-0.132554	-0.024015	0.046543
C_2H_5OH -Ne	0.000109	-3.962573502	-0.000078	-0.132554	-0.001615	0.064701
C_2H_5OH -H_2	0.000206	-3.68613278	-0.000044	-0.132554	-0.001042	0.065257
C_2H_5OH -n-C_3H_8	0.0228	-1.642065153	-0.029806	-0.132554	-0.051803	0.029377
C_2H_5OH- n-C_4H_{10}	0.0815	-1.088842391	-0.05899	-0.132554	-0.079148	0.016624
C_2H_5OH -CO_2	0.00689	-2.161780778	-0.007489	-0.132554	-0.021915	0.0481065
VDUD solvent-solute	**x_{solute}**	**log x_{solute}**	**P11*E19 (J)**	**P22*E19P1 (J)**	**2-GLP*E19 (J)**	**w′ (GLP)*E19 (J)**
CH_3OH- CH_4	0.000871	-3.059981845	-0.006385	-0.047341	-0.01554	0.011323
CH_3OH-Ar	0.000447	-3.349692477	-0.003117	-0.047341	-0.008755	0.016474
CH_3OH-H_2	0.000161	-3.793174124	-0.000044	-0.047341	-0.00082	0.0228725
CH_3OH-N_2	0.000276	-3.559090918	-0.001535	-0.047341	-0.006383	0.018055
CH_3OH-O_2	0.000415	-3.381951903	-0.00293	-0.047341	-0.009973	0.0151625
CH_3OH-CO	0.000327	-3.485452247	-0.001976	-0.047341	-0.007472	0.0171865
CH_3OH-C_2H_4	0.0047	-2.327902142	-0.018977	-0.047341	-0.028618	0.004541
CH_3OH-C_2H_6	0.00393	-2.40560745	-0.008562	-0.047341	-0.017595	0.0103565
CH_3OH-Ne	0.0000804	-4.094743951	-0.000078	-0.047341	-0.001306	0.0224035
CH_3OH-n-C_3H_8	0.0115	-1.93930216	-0.029806	-0.047341	-0.035302	0.0032715
CH_3OH-n-C_4H_{10}	0.0398	-1.400116928	-0.05899	-0.047341	-0.050071	0.0030945
CH_3OH-CO_2	0.00639	-2.194499142	-0.007489	-0.047341	-0.016616	0.010799

Table A9-2. The obtained unlike pair potentials and interchange energy calculated by method VDUD and the unlike London pair potential and the experimental solubility (x_{solute}) for gases in liquids at 298.15 K, 101.325 kPa.

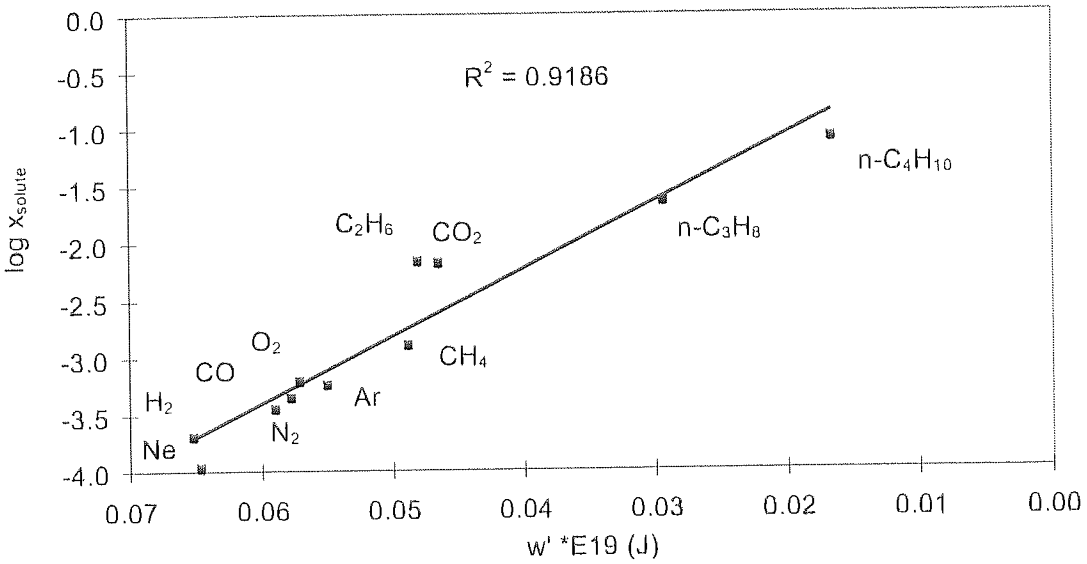

Figure A9.8. Solubilities of gases in **ethanol** at 298.15 K, 101.325 kPa as a function of the interchange energy (w′) calculated by method VDUD and the unlike London pair potential.

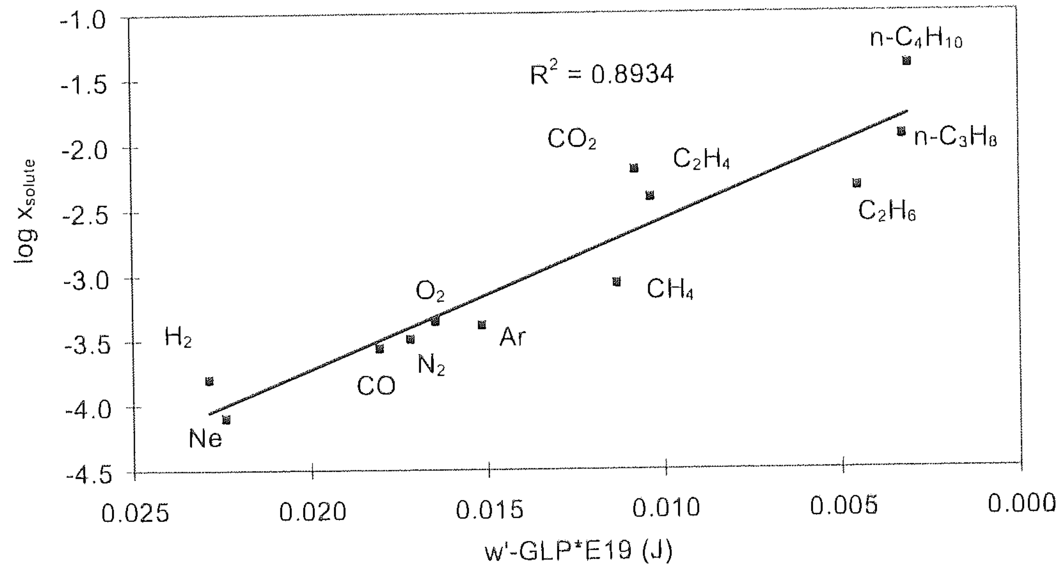

Figure A9.9. Solubilities of gases in **methanol** at 298.15 K, 101.325 kPa as a function of the interchange energy (w′) calculated by method VDUD and the unlike London pair potential.

A9.1.3 Results of heat of vaporization calculations

VDUD solvent-solute	x_{solute}	log x_{solute}	P12-GLP*E19 (J)	P12-GM*E19 (J)
C_6H_6-CH_4	0.00209	-2.67985371	-0.023337	-0.027543315
C_6H_6-Ar	0.000882	-3.05453141	-0.013063	-0.019988712
C_6H_6-N_2	0.000445	-3.35163999	-0.011256	-0.015270226
C_6H_6-O_2	0.00081	-3.09151498	-0.017782	-0.022679299
C_6H_6-CO	0.00065	-3.18708664	-0.01288	-0.017150994
C_6H_6-C_2H_4	0.01185	-1.92628165	-0.043968	-0.047590891
C_6H_6-H_2	0.0002591	-3.58653259	-0.000317	-0.000751399
C_6H_6-Ne	0.0001151	-3.93892468	-0.001175	-0.001840543
C_6H_6-CO_2	0.00912	-2.04000516	-0.025425	-0.030137239
C_6H_6-C_2H_6	0.0149	-1.82681373	-0.023343	-0.027022509
C_6H_6-n-C_3H_8	0.0573	-1.24184538	-0.05673	-0.058710161
VDUD solvent-solute	x_{solute}	log x_{solute}	**P12-GLP*E19 (J)**	**P12-GM*E19 (J)**
CCl_4-CH_4	0.002856	-2.5442418	-0.025392	-0.027083657
CCl_4-Ar	0.00135	-2.86966623	-0.014764	-0.019666825
CCl_4-N_2	0.000641	-3.19314197	-0.012626	-0.01502331
CCl_4-O_2	0.0012	-2.92081875	-0.019567	-0.02231174
CCl_4-CO	0.000865	-3.06298389	-0.014468	-0.016877649
CCl_4-C_2H_4	0.0148	-1.82973828	-0.045694	-0.046803446
CCl_4-H_2	0.0003225	-3.49147028	-0.000368	-0.000738951
CCl_4-C_2H_6	0.0211	-1.67571754	-0.025506	-0.026574839
CCl_4-n-C_3H_8	0.0731	-1.13608262	-0.057685	-0.057737536
CCl_4-n-C_4H_{10}	0.339	-0.4698003	-0.07026	-0.07115318
CCl_4-CO_2	0.0106	-1.97469413	-0.027546	-0.029634898
VDUD solvent-solute	x_{solute}	log x_{solute}	**P12-GLP*E19 (J)**	**P12-GM*E19 (J)**
C_2H_5OH-CH_4	0.00128	-2.89279003	-0.023226	-0.031458075
C_2H_5OH-Ar	0.0006257	-3.20363385	-0.012427	-0.022829728
C_2H_5OH-N_2	0.000357	-3.44733178	-0.010518	-0.017440599
C_2H_5OH-O_2	0.0005825	-3.23470407	-0.017798	-0.025902732
C_2H_5OH-CO	0.000449	-3.34775366	-0.012212	-0.019588683
C_2H_5OH-H_2	0.000206	-3.68613278	-0.000251	-0.000858182
C_2H_5OH-Ne	0.000109	-3.9625735	-0.000997	-0.002102108
C_2H_5OH-C_2H_6	0.00666	-2.17652577	-0.02207	-0.030863247
C_2H_5OH-n-C_3H_8	0.228	-0.64206515	-0.057489	-0.067054698
C_2H_5OH-n-C_4H_{10}	0.615	-0.21112488	-0.074106	-0.082633891
C_2H_5OH-CO_2	0.00689	-2.16178078	-0.02504	-0.03441655

Table A9-3. The obtained unlike pair potentials calculated by method VDUD and the experimental solubility (x_{solute}) for gases in liquids at 298.15 K, 101.325 kPa.

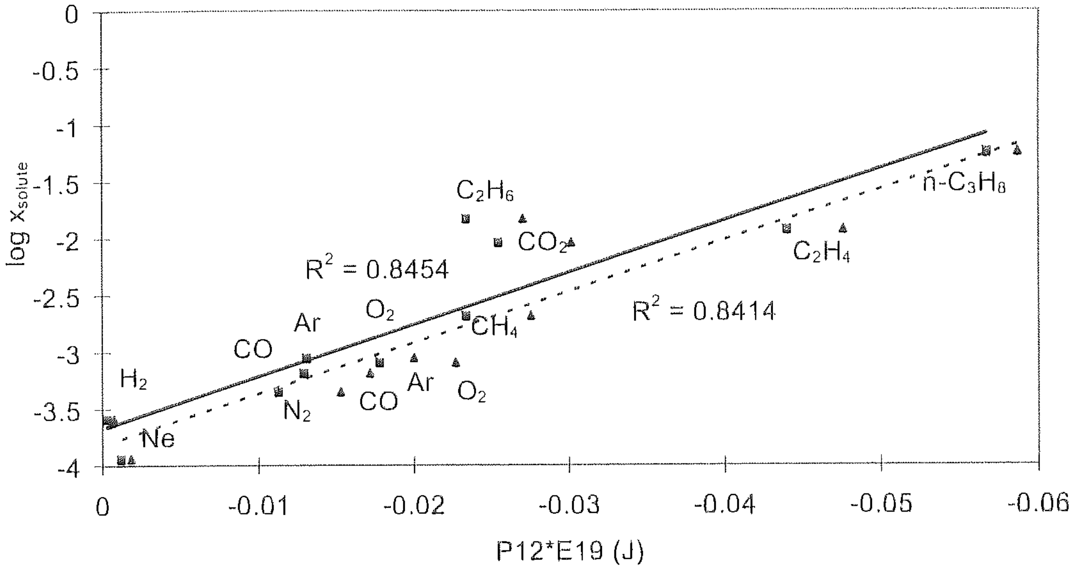

Figure A9.10. Solubilities of gases in **benzene** at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP, ■ points and — line) and the geometric mean unlike pair potential (P12-GM, ▲ points and -- line) calculated by method VDUD.

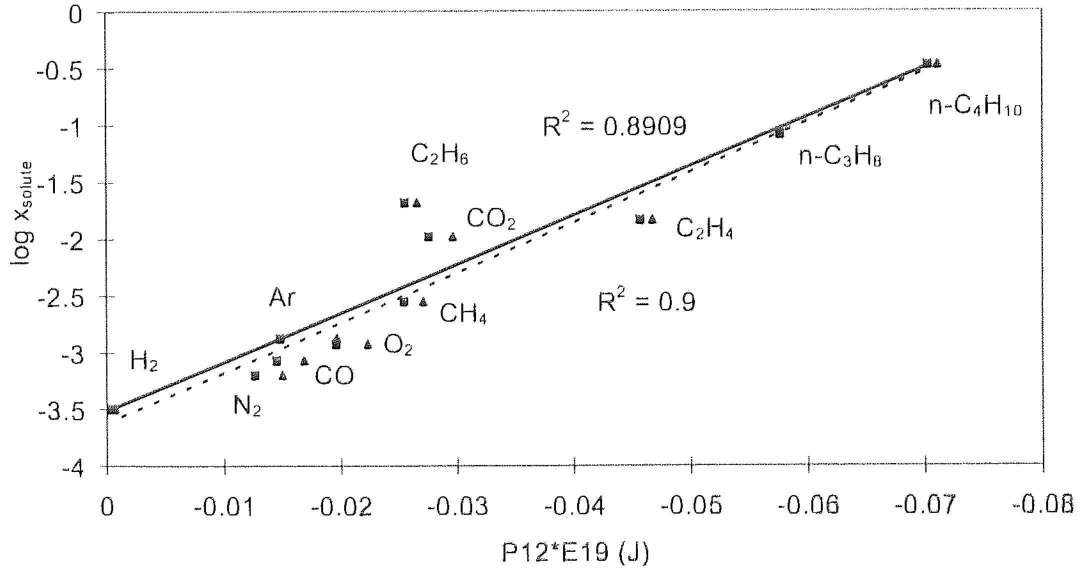

Figure A9.11. Solubilities of gases in **carbon tetrachloride** at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential

(P12-GLP, ■ points and – line) and the geometric mean unlike pair potential (P12-GM, ▲ points and -- line) calculated by method VDUD.

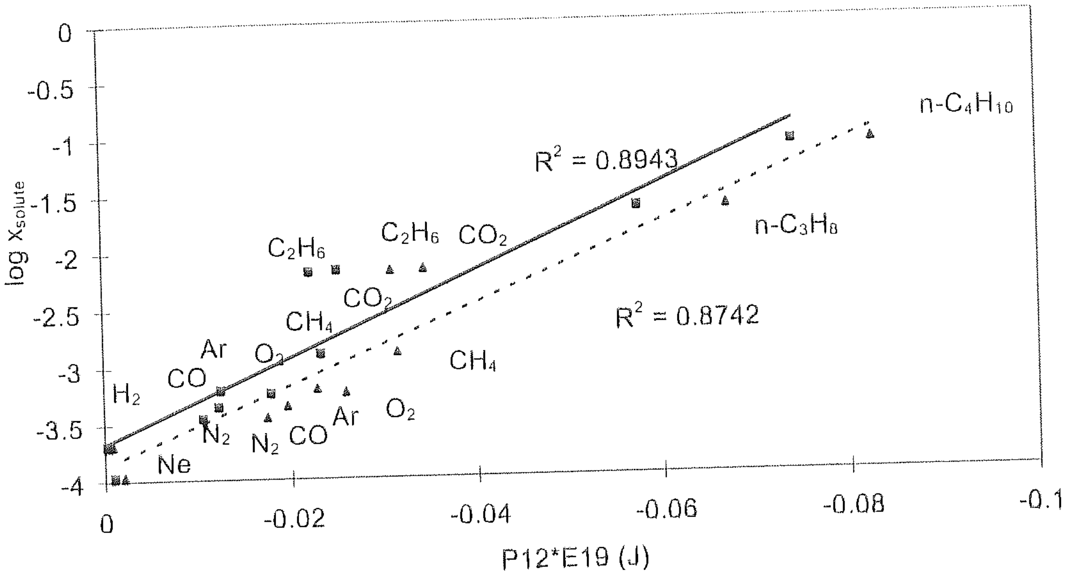

Figure A9.12. Solubilities of gases in **ethanol** at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP, ■ points and – line) and the geometric mean unlike pair potential (P12-GM, ▲ points and -- line) calculated by method VDUD.

A9.2 Results of VDUD calculations for a single solute dissolved in a series of solvents

A9.2.1 Results of molar volume calculations

VDUD solvent-solute	x_{solute}	log x_{solute}	**P12-GLP*E19 (J)**
C_6H_6-CH_4	0.00209	-2.679853714	-2.257200E-02
c-C_6H_{12}-CH_4	0.00327	-2.485452247	-2.161300E-02
CS_2-CH_4	0.001309	-2.883060353	-2.339200E-02
H_2O-CH_4	0.00002548	-4.593800576	-1.203300E-02
CCl_4-CH_4	0.002856	-2.544241797	-2.065800E-02
CH_3OH-CH_4	0.000871	-3.059981845	-1.554E-02
C_2H_5OH-CH_4	0.00128	-2.89279003	-2.0601E-02
C_3H_7OH-CH_4	0.00156	-2.804100348	-2.5621E-02
VDUD solvent-solute	x_{solute}	log x_{solute}	**P12-GLP*E19 (J)**
C_6H_6-Ar	0.00882	-3.054531415	-1.210000E-02
c-C_6H_{12}-Ar	0.00114	-2.943095149	-1.155300E-02
CS_2-Ar	0.00135	-3.31309573	-1.384000E-02
H_2O-Ar	0.0004863	-4.598771833	-7.399000E-03
CCl_4-Ar	0.00002519	-2.869666232	-1.173800E-02
CH_3OH-Ar	0.000447	-3.349692477	-0.08755E-02
C_2H_5OH-Ar	0.0006257	-3.349692477	-1.068E-02
C_3H_7OH-Ar	0.000777	-3.109578981	-1.2092E-02
$CHCl_3$-Ar	0.000592	-3.227678293	-1.008500E-02
VDUD solvent-solute	x_{solute}	log x_{solute}	**P12-GLP*E19 (J)**
C_6H_6-n-C_3H_8	0.0573	-1.241845378	-0.056392
c-C_6H_{12}- n-C_3H_8	0.0910	-1.040958608	-0.052912
CS_2- n-C_3H_8	0.0813	-1.350665141	-0.052065
H_2O- n-C_3H_8	0.0446	-4.563519305	-0.024876
CCl_4- n-C_3H_8	0.00002732	-1.089909454	-0.047485
CH_3OH-n-C_3H_8	0.0115	-1.93930216	-0.035302
C_2H_5OH-n-C_3H_8	0.0228	-1.642065153	-0.051803

Table A9-4. The obtained unlike pair potentials calculated by method VDUD and the experimental solubility (x_{solute}) for gases in liquids at 298.15 K, 101.325 kPa (continued over).

VDUD solvent-solute	x_{solute}	log x_{solute}	P12-GLP*E19 (J)
C_6H_6-CO_2	0.00912	-1.241845378	-0.056392
c-C_6H_{12}-CO_2	0.00759	-1.040958608	-0.052912
CS_2-CO_2	0.00328	-1.350665141	-0.052065
H_2O-CO_2	0.0006116	-3.21353252	-0.024876
CCl_4-CO_2	0.0106	-1.089909454	-0.047485
CH_3OH-CO_2	0.00639	-1.93930216	-0.035302
C_2H_5OH-CO_2	0.00689	-1.642065153	-0.051803
C_3H_7OH-CO_2	0.00772	-2.1123827	-0.027072
$CHCl_3$- CO_2	0.0128	-1.89279003	-0.0710120
VDUD solvent-solute	x_{solute}	log x_{solute}	P12-GLP*E19 (J)
C_6H_6-H_2	0.0002591	-3.586532587	-1.282000E-03
c-C_6H_{12}- H_2	0.000414	-3.382999659	-1.294000E-03
CS_2- H_2	0.0001593	-3.797784224	-1.418000E-03
H_2O- H_2	0.00001411	-4.850472986	-5.980000E-04
CCl_4- H_2	0.0003225	-3.491470281	-1.311000E-03
CH_3OH-H_2	0.000161	-3.491470281	-8.2E-04
C_2H_5OH-H_2	0.000206	-3.688246139	-1.042E-03
C_3H_7OH- H_2	0.000231	-3.63638802	-1.212E-03
$CHCl_3$- H_2	0.000022	-3.657577319	-1.116000E-03
VDUD solvent-solute	x_{solute}	log x_{solute}	P12-GLP*E19 (J)
C_6H_6-N_2	0.000445	-3.351639989	-9.336000E-03
c-C_6H_{12}- N_2	0.000768	-3.11463878	-9.061000E-03
CS_2- N_2	0.0001593	-3.654626269	-1.028000E-02
H_2O- N_2	0.00001183	-4.927015255	-4.993000E-03
CCl_4- N_2	0.000641	-3.19314197	-9.053000E-03
CH_3OH-N_2	0.000276	-3.559090918	-0.6383E-02
C_2H_5OH-N_2	0.000357	-3.447331784	-0.8036E-02
C_3H_7OH - N_2	0.000402	-3.395773947	-0.9369E-02
$CHCl_3$ - N_2	0.000445	-3.351639989	-0.7739E-02
VDUD solvent-solute	x_{solute}	log x_{solute}	P12-GLP*E19 (J)
C_6H_6-O_2	0.000810	-3.091514981	-1.403200E-02
c-C_6H_{12}- O_2	0.00123	-2.910094889	-1.343500E-02
CS_2- O_2	0.000439	-3.35753548	-1.519200E-02
H_2O- O_2	0.00002293	-4.639595945	-8.024000E-03
CCl_4- O_2	0.0012	-2.920818754	-1.316700E-02
CH_3OH-O_2	0.000415	-3.381951903	-0.9973E-02
C_2H_5OH-O_2	0.0005825	-3.23470407	-1.2701E-02
C_3H_7OH - O_2	0.000503	-3.298432015	-1.5141E-02

Table A9-4. The obtained unlike pair potentials calculated by method VDUD and the experimental solubility (x_{solute}) for gases in liquids at 298.15 K, 101.325 kPa (continued over).

VDUD solvent-solute	x_{solute}	**log** x_{solute}	**P12-GLP*E19 (J)**
C_6H_6-CO	0.000650	-3.187086643	-1.082800E-02
c-C_6H_{12}- CO	0.000999	-3.000434512	-1.054500E-02
CS_2- CO	0.000360	-3.443697499	-1.187700E-02
H_2O- CO	0.0000172	-4.764471553	-5.847000E-03
CCl_4- CO	0.000865	-3.062983893	-1.047900E-02
CH_3OH-CO	0.000327	-3.485452247	-0.7472E-02
C_2H_5OH-CO	0.000449	-3.347753659	-0.9449E-02
C_3H_7OH - CO	0.0005193	-3.284581677	-1.1099E-02
$CHCl_3$ - CO	0.000665	-7.31572	-8.959000E-03
VDUD solvent-solute	x_{solute}	**log** x_{solute}	**P12-GLP*E19 (J)**
C_6H_6-C_2H_6	0.0149	-1.826813732	-2.712500E-02
c-C_6H_{12}- C_2H_6	0.0233	-1.632644079	-2.630800E-02
CS_2- C_2H_6	0.0107	-1.970616222	-2.713300E-02
H_2O- C_2H_6	0.0000340	-4.468521083	-1.270500E-02
CCl_4- C_2H_6	0.0211	-1.675717545	-2.479700E-02
CH_3OH-C_2H_6	0.00393	-2.40560745	-1.7595E-02
C_2H_5OH-C_3H_6	0.00666	-2.176525771	-2.4015E-02
VDUD solvent-solute	x_{solute}	**log** x_{solute}	**P12-GLP*E19 (J)**
H_2O- n-C_4H_{10}	0.00002244	-4.648977147	-0.03438
CCl_4- n-C_4H_{10}	0.3390	-0.469800302	-0.065446
CH_3OH-n-C_4H_{10}	0.0398	-1.400116928	-0.050071
C_2H_5OH-n-C_4H_{10}	0.0815	-1.088842391	-0.079148

Table A9-4. The obtained unlike pair potentials calculated by method VDUD and the experimental solubility (x_{solute}) for gases in liquids at 298.15 K, 101.325 kPa.

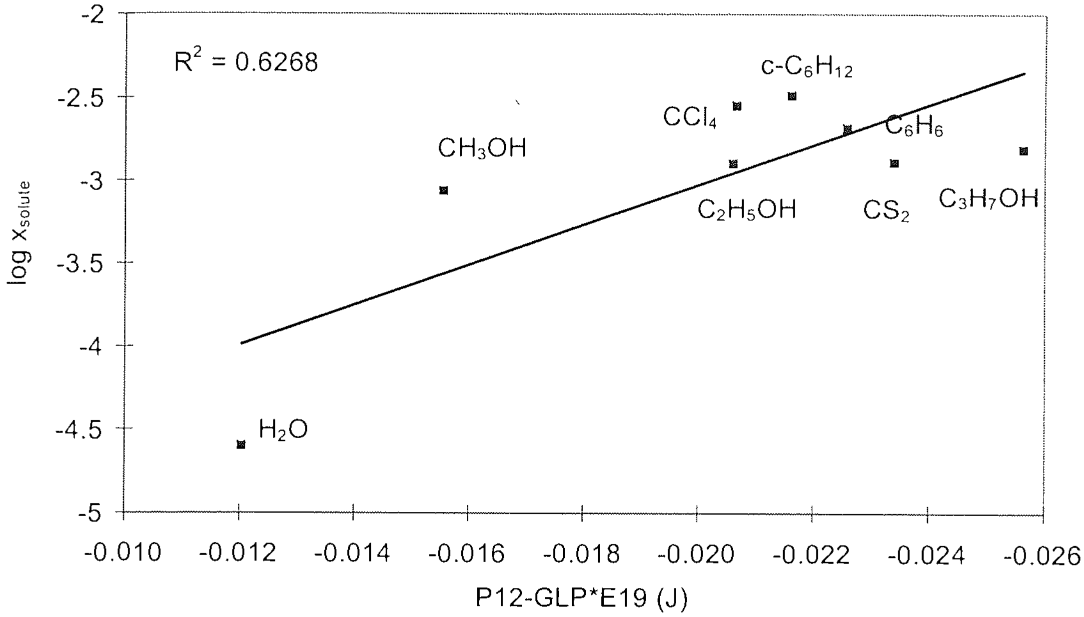

Figure A9.13. Solubilities of **methane** in solvents at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP) calculated by method VDUD.

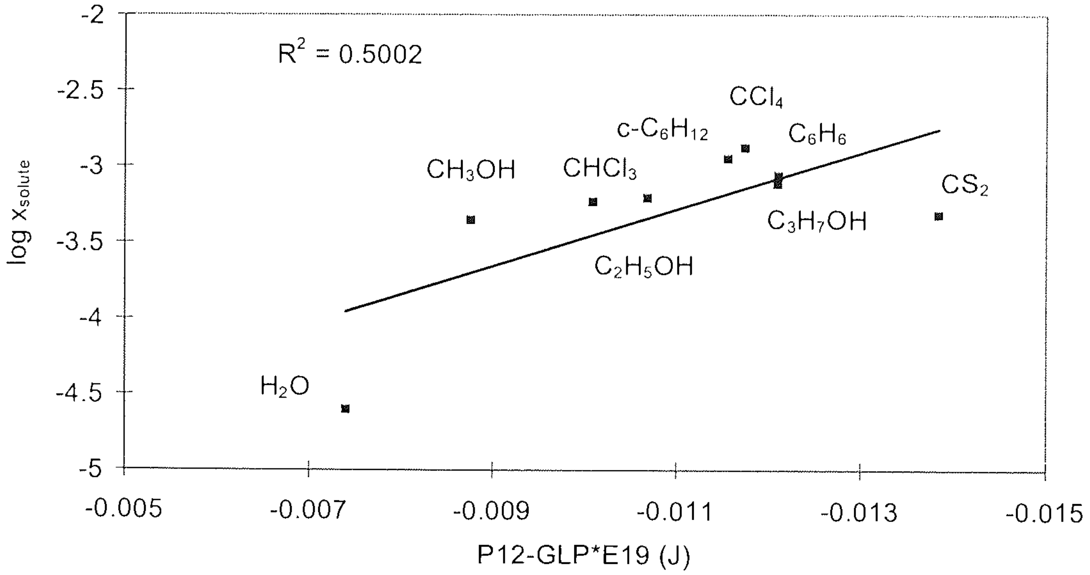

Figure A9.14. Solubilities of **argon** in solvents at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP) calculated by method VDUD.

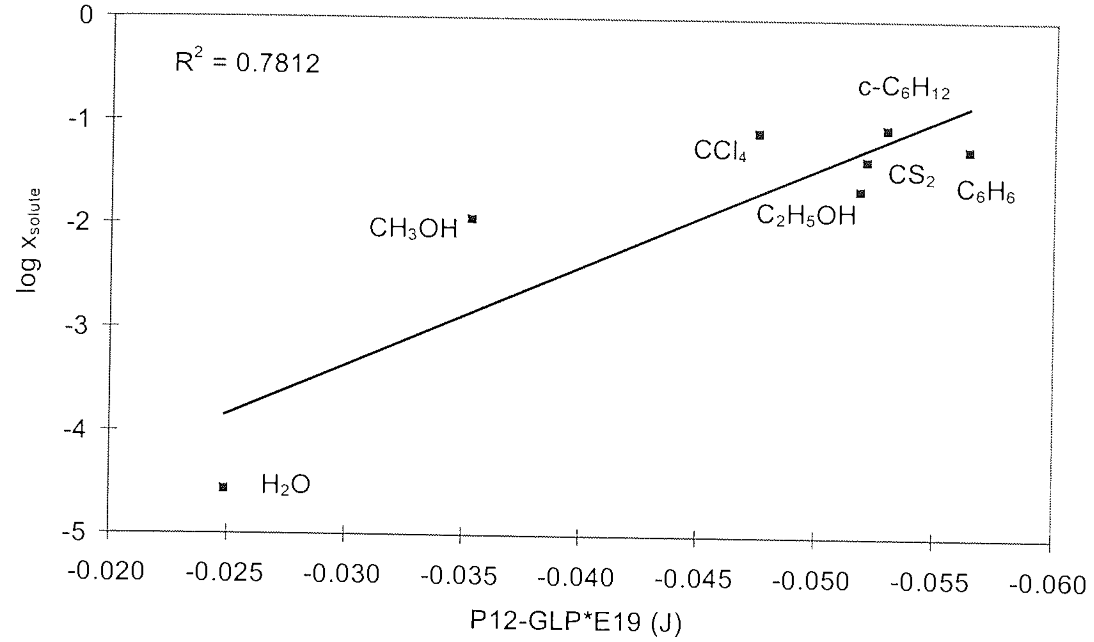

Figure A9.15. Solubilities of **n-propane** in solvents at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP) calculated by method VDUD.

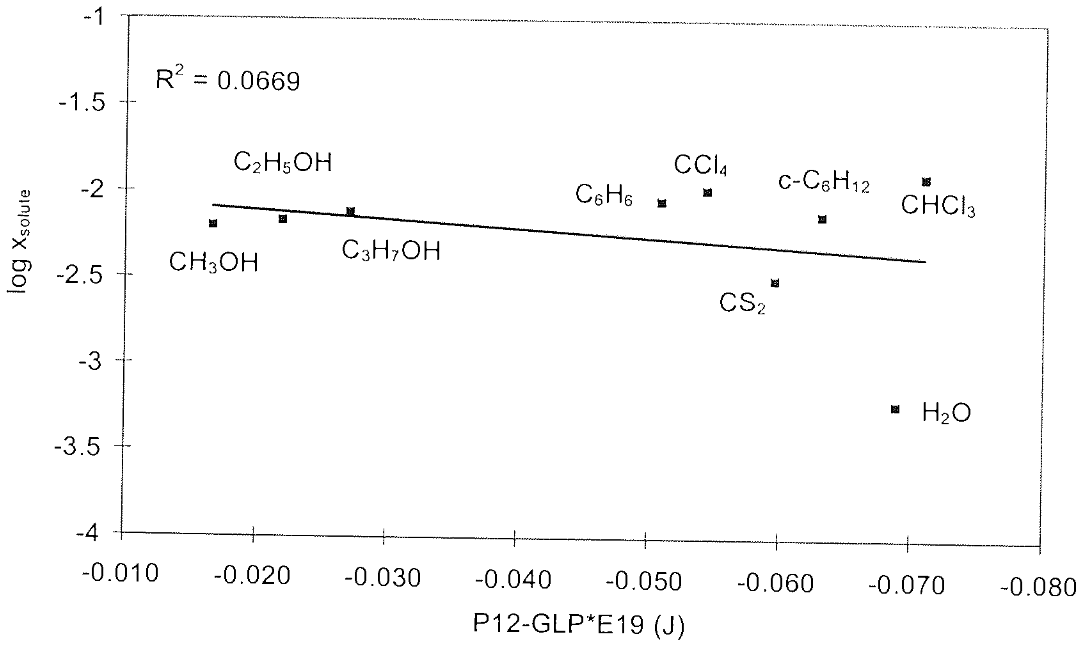

Figure A9.16. Solubilities of **carbon dioxide** in solvents at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP) calculated by method VDUD.

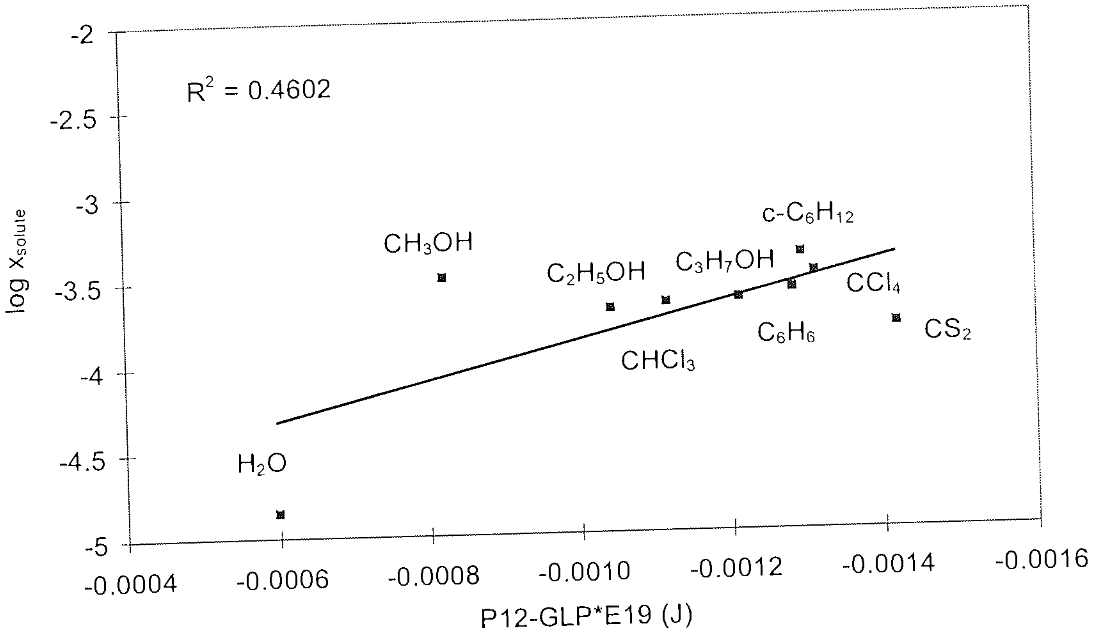

Figure A9.17. Solubilities of **hydrogen** in solvents at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP) calculated by method VDUD.

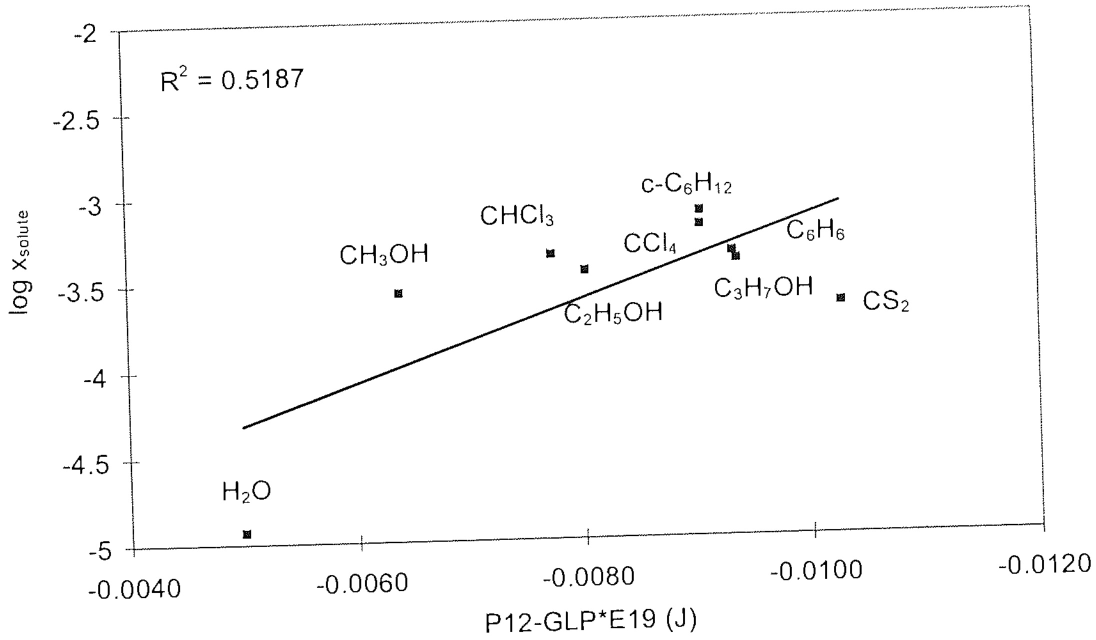

Figure A9.18. Solubilities of **nitrogen** in solvents at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP) calculated by method VDUD.

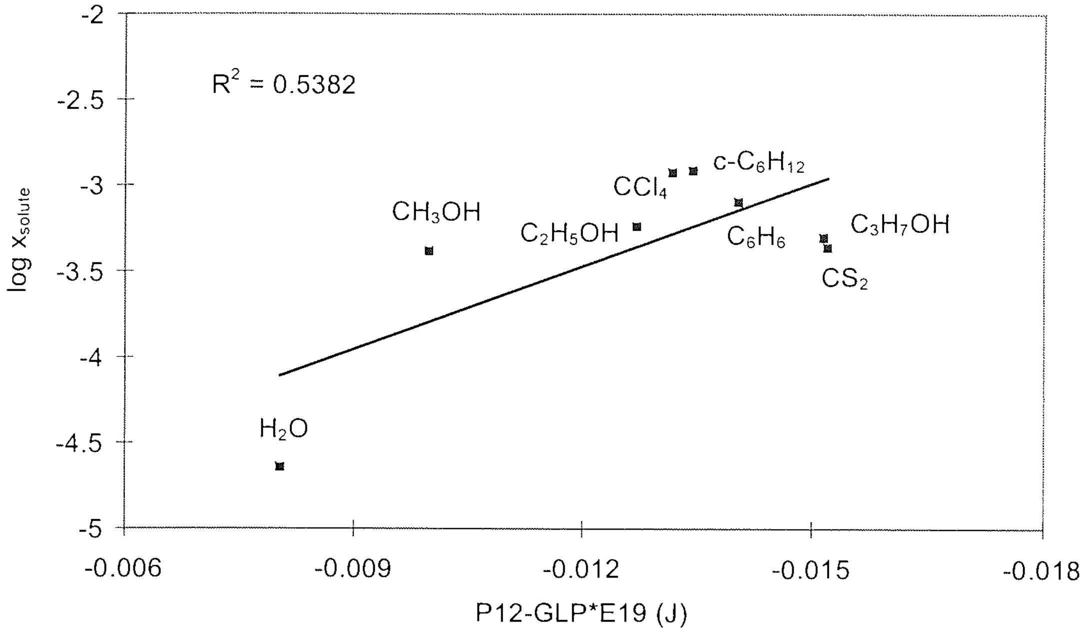

Figure A9.19. Solubilities of **oxygen** in solvents at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP) calculated by method VDUD.

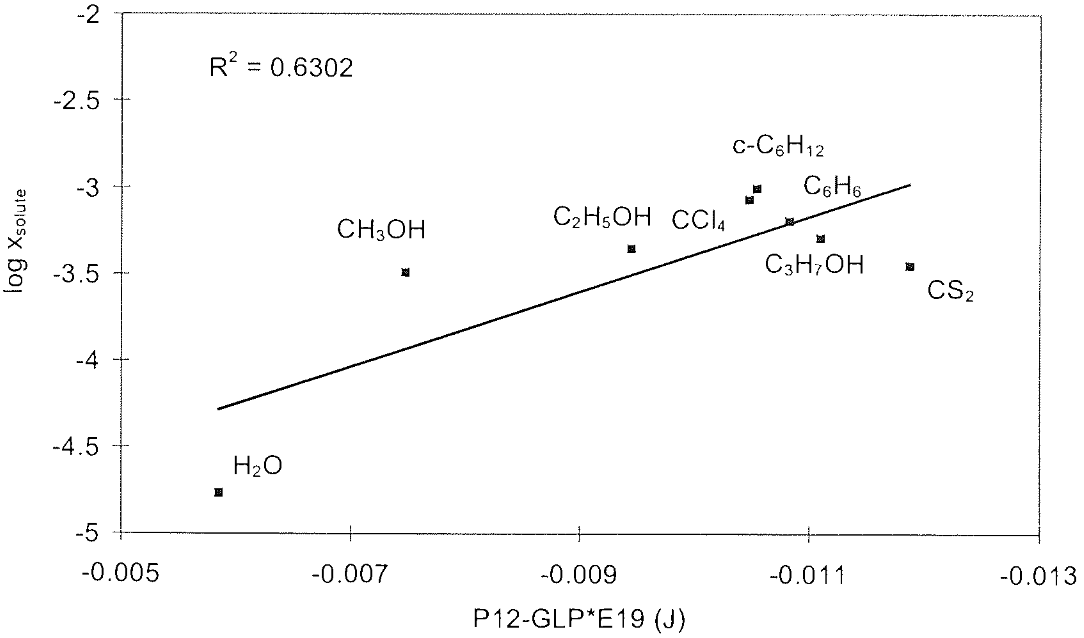

Figure A9.20. Solubilities of **carbon monoxide** in solvents at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP) calculated by method VDUD.

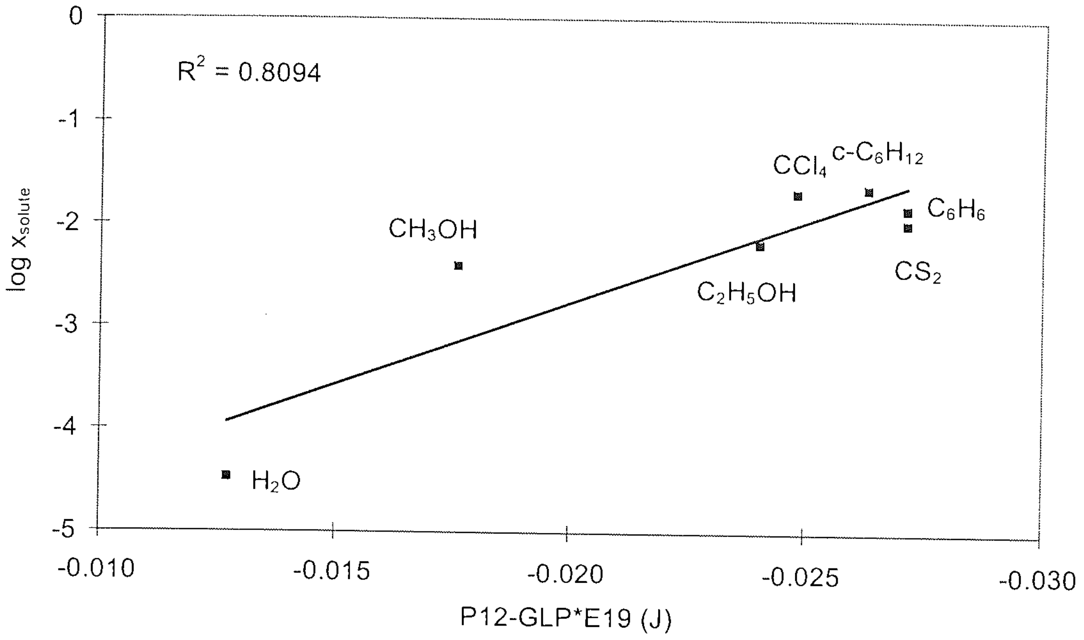

Figure A9.21. Solubilities of **ethane** in solvents at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP) calculated by method VDUD.

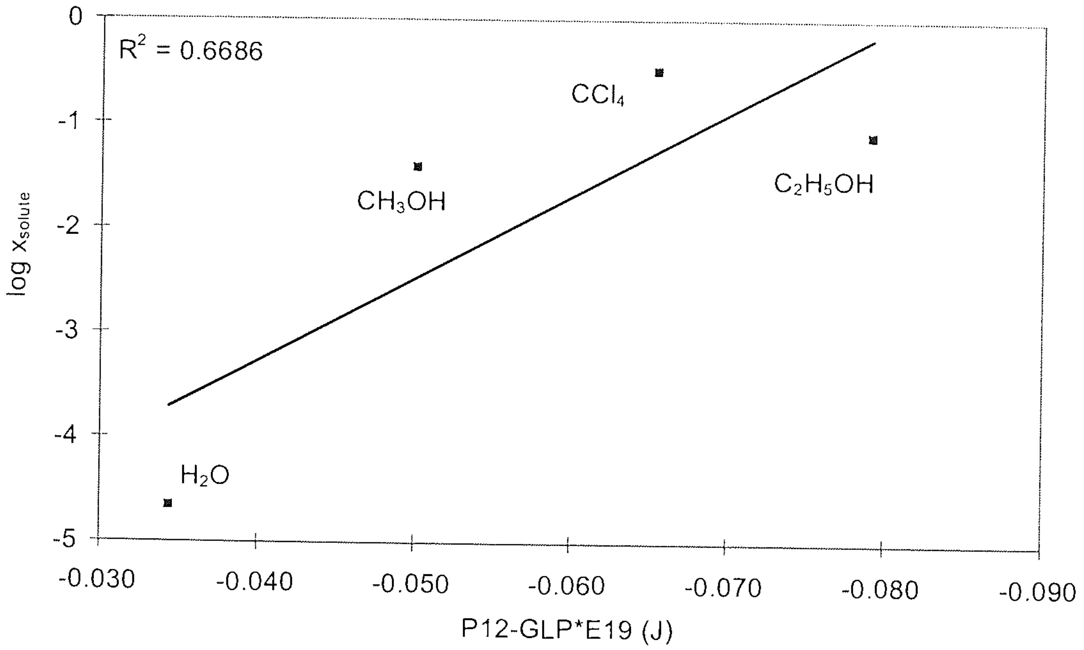

Figure A9.22. Solubilities of **n-butane** in solvents at 298.15 K, 101.325 kPa a function of the generalized unlike London pair potential (P12-GLP) calculated by method VDUD.

A9.2.2 Interchange energy

VDUD solvent-solute	x_{solute}	log x_{solute}	P11*E19 (J)	P22*E19 (J)	P12-GLP*E19 (J)	w′ (GLP)*E19 (J)
C_6H_6-CH_4	0.00209	-2.679853714	-0.123816	-0.006385	-2.257200E-02	0.0425285
c-C_6H_{12}-CH_4	0.00327	-2.485452247	-0.098488	-0.006385	-2.161300E-02	0.0308235
CS_2-CH_4	0.001309	-2.883060353	-0.09249	-0.006385	-2.339200E-02	0.0260455
H_2O-CH_4	0.00002548	-4.593800576	-0.030407	-0.006385	-1.203300E-02	0.006363
CCl_4-CH_4	0.002856	-2.544241797	-0.075741	-0.006385	-2.065800E-02	0.020405
CH_3OH-CH_4	0.000871	-3.059981845	-0.047341	-0.006385	-1.554E-02	0.011323
C_2H_5OH-CH_4	0.00128	-2.89279003	-0.132554	-0.006385	-2.0601E-02	0.0488685
C_3H_7OH-CH_4	0.00156	-2.804100348	-0.204653	-0.006385	-2.5621E-02	0.079898

Table A9-5. The obtained unlike pair potentials and interchange energy calculated by method VDUD and the unlike London pair potential and the experimental solubility (x_{solute}) for methane in liquids at 298.15 K, 101.325 kPa.

Table A9-5 shows the results of the interchange energy calculations for methane using the unlike geometric mean potential or the generalized unlike London pair potential. Figures 4.14 (chapter 4) shows the plots.

Similarly, Table A9-6 shows the results of the interchange energy calculations for propane and carbon dioxide using the different options of heat of vaporization or molar volume and the unlike geometric mean potential or the generalized unlike London pair potential. The interchange energy for carbon dioxide obtained from heat of vaporization is shown as well. The interchange energy (w′) has been divided by k_BT to obtain dimensionless numbers. Figures 4.15 and 4.16 (chapter 4) show the plots.

Hvap	Hvap	Hvap	Hvap	Hvap	Hvap	Hvap	Hvap	Hvap	Hvap	Hvap
solvent-solute	P11*E19 (J)	P22*E19 (J)	P12-GLP*E19 (J)	w'-GLP*E19 (J)	z w'-GLP *E19 (J)	P12-GM*E19 (J)	w'-GM*E19 (J)	z w'-GM/ k_B T	x_{solute}	log x(solute)
c-C_6H_{12}-C_3H_8	-0.091765	-0.03663	-0.057121	0.0070765	1.890989035	-0.057977167	0.006220333	1.662203147	0.0910	-1.040958608
CCl_4 -C_3H_8	-0.091008	-0.03663	-0.057685	0.006134	1.639133292	-0.057737536	0.006081464	1.625094626	0.0813	-1.089909454
C_6H_6 -C_3H_8	-0.0941	-0.03663	-0.05673	0.008635	2.307452882	-0.058710161	0.006654839	1.778312394	0.0573	-1.241845378
CS_2 -C_3H_8	-0.075917	-0.03663	-0.052358	0.0039155	1.04630362	-0.052733668	0.003539832	0.945917339	0.0446	-1.350665141
CH_3OH -C_3H_8	-0.107612	-0.03663	-0.055461	0.01666	4.451900985	-0.062783975	0.009337025	2.495048575	0.0115	-1.93930216
C_2H_5OH -C_3H_8	-0.122746	-0.03663	-0.057489	0.022199	5.932037814	-0.067053605	0.012634395	3.37617493	0.0228	-1.642065153
H_2O -C_3H_8	-0.127049	-0.03663	-0.048183	0.0336565	8.993721819	-0.068218801	0.013620699	3.639735975	0.0002732	-4.563519305
c-C_6H_{12} -CO2	-0.091765	-0.009652	-0.025736	0.0249715	6.67290789	-0.029757894	0.020949606	5.598173589	0.00759	-2.119758224
CS_2 - CO_2	-0.075917	-0.009652	-0.026399	0.0163845	4.378281614	-0.027066567	0.015716933	4.199893724	0.00328	-2.484126156
H_2O - CO_2	-0.12705	-0.009652	-0.024664	0.043687	11.67408153	-0.035018375	0.033332625	8.907175588	0.0006116	-3.213532523
$CHCl_3$ - CO_2	-0.088039	-0.009652	-0.027079	0.0217655	5.816197533	-0.029147493	0.019697007	5.263452865	0.0128	-1.89279003
CH_3OH - CO_2-	-0.107612	-0.00965	-0.026008	0.032623	8.71754897	-0.03222508	0.02640592	7.056214883	0.00639	-2.194499142
C_3H_7OH - CO_2	-0.13698	-0.009652	-0.026624	0.046692	12.47708048	-0.036361119	0.036954881	9.87511837	0.00772	-2.1123827
C_6H_6 - CO_2	-0.0941	-0.009652	-0.025425	0.026451	7.068261282	-0.030137239	0.021738761	5.809052199	0.00912	-2.040005162
CCl_4 - CO_2	-0.091008	-0.009652	-0.027546	0.022783	6.088094847	-0.029634898	0.020694102	5.529897452	0.0106	-1.974694135
C_2H_5OH - CO_2	-0.122746	-0.009652	-0.02504	0.041158	10.99827976	-0.03441655	0.03178145	8.492669236	0.00689	-2.161780778
mol. vol.	mol. vol.	mol. vol.	mol. vol.	mol. vol.	mol. vol.	mol. vol.	mol. vol.	mol. vol.	mol. vol.	mol. vol.
solvent-solute	P11*E19 (J)	P22*E19 (J)	P12-GLP*E19 (J)	w'-GLP*E19 (J)	z w'-GLP *E19 (J)	P12-GM*E19 (J)	w'-GM*E19 (J)	z w'-GM/ k_B T	x_{solute}	log x(solute)
c-C_6H_{12} -C_3H_8	-0.098488	-0.029806	-0.052912	0.011235	3.002227345	-0.054180562	0.009966438	2.663240933	0.0910	-1.040958608
CCl_4 -C_3H_8	-0.075741	-0.029806	-0.047485	0.0052885	1.413197981	-0.047513538	0.005259962	1.405572162	0.0813	-1.089909454
C_6H_6 -C_3H_8	-0.123816	-0.029806	-0.056392	0.020419	5.456384527	-0.060749154	0.016061846	4.292061741	0.0573	-1.241845378
CS_2 -C_3H_8	-0.09249	-0.029806	-0.052065	0.009083	2.427167866	-0.052504828	0.008643172	2.309636671	0.0446	-1.350665141
CH_3OH -C_3H_8	-0.047341	-0.029806	-0.035302	0.0032715	0.87421333	-0.03756389	0.00100961	0.269788891	0.0115	-1.93930216
C_2H_5OH -C_3H_8	-0.132554	-0.029806	-0.051803	0.029377	7.850149775	-0.062856221	0.018323779	4.896497574	0.0228	-1.642065153
H_2O -C_3H_8	-0.030407	-0.029806	-0.024876	0.0052305	1.397699166	-0.030105	1.49972E-06	0.000400756	0.0002732	-4.563519305

Table A9-6. The results of the interchange energy calculations for **propane** and **carbon dioxide** using the different options of heat of vaporization or molar volume and the geometric mean unlike potential or the generalized unlike London potential.

A9.3 Results of VNUN, VDUN, and VDUD methods

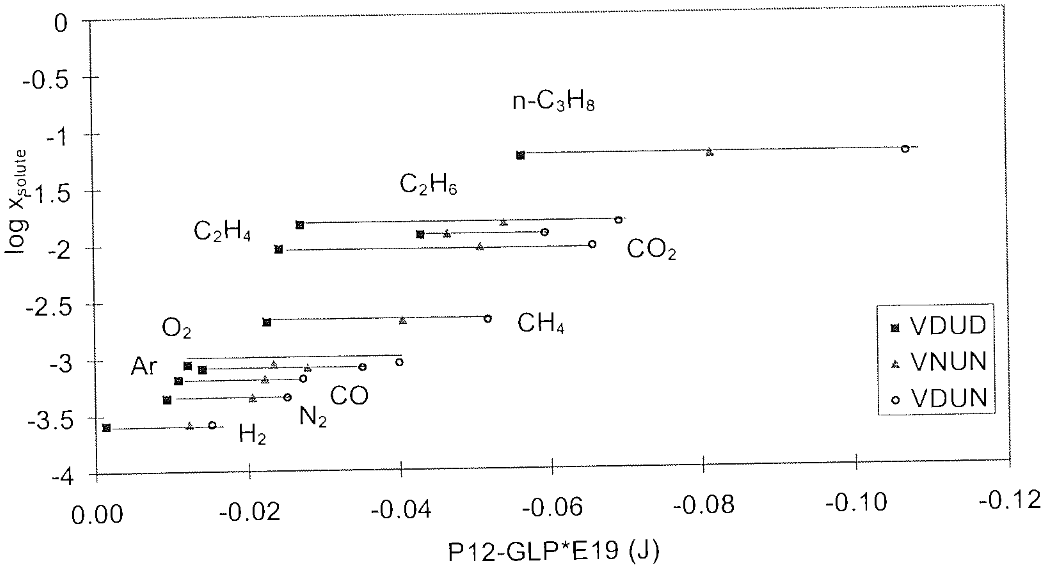

Figure A9.23. Solubilities of gases in **benzene** at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP) calculated by methods VNUN, VDUN, and VDUD.

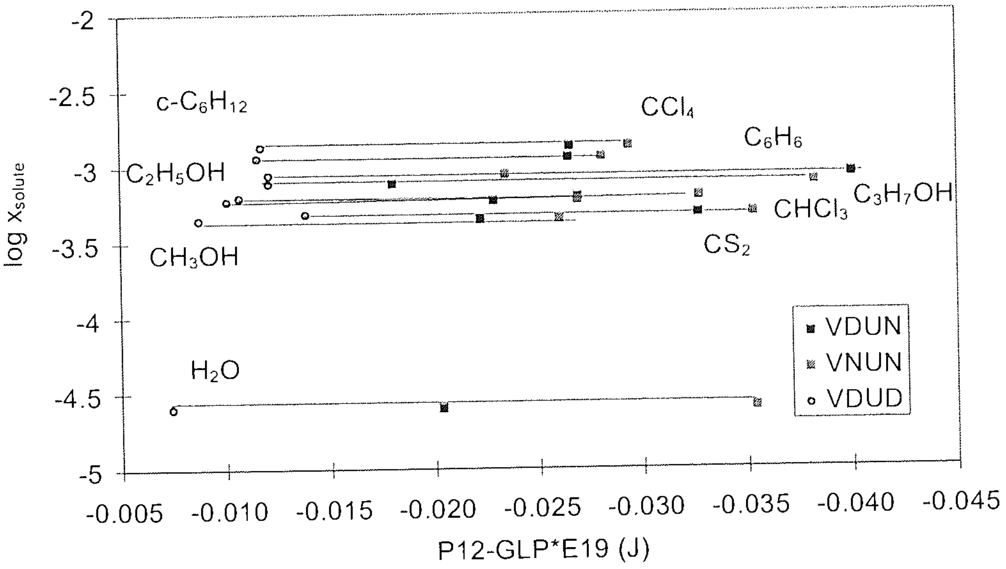

Figure A9.24. Solubilities of **argon** in solvents at 298.15 K, 101.325 kPa as a function of the generalized unlike London pair potential (P12-GLP) calculated by methods VNUN, VDUN, and VDUD.

Appendix 10 - Results of temperature correlation of the pair potentials

The results obtained of the performed calculations are shown in Table A10-1. In Table A10-1 the first column shows the mixture, the solute's name first, then follows the experimental data in columns 2 and 3. The temperature first, then the solubility (liquid mole fraction of the solute (component 1)) is in column three. The experimental data are from Fogg and Gerrard (1991) or Solubility Data Series, vol. 24. The natural logarithm of the solubility is in column four. Then follows the predicted results in the next columns. The equilibrium separation for the solute, then the equilibrium separation for the solvent, the like pair potential for the solute, and the like pair potential for the solvent. The last two columns contain the unlike pair potential data as calculated by the London combining rule and the geometric mean combining rule, respectively.

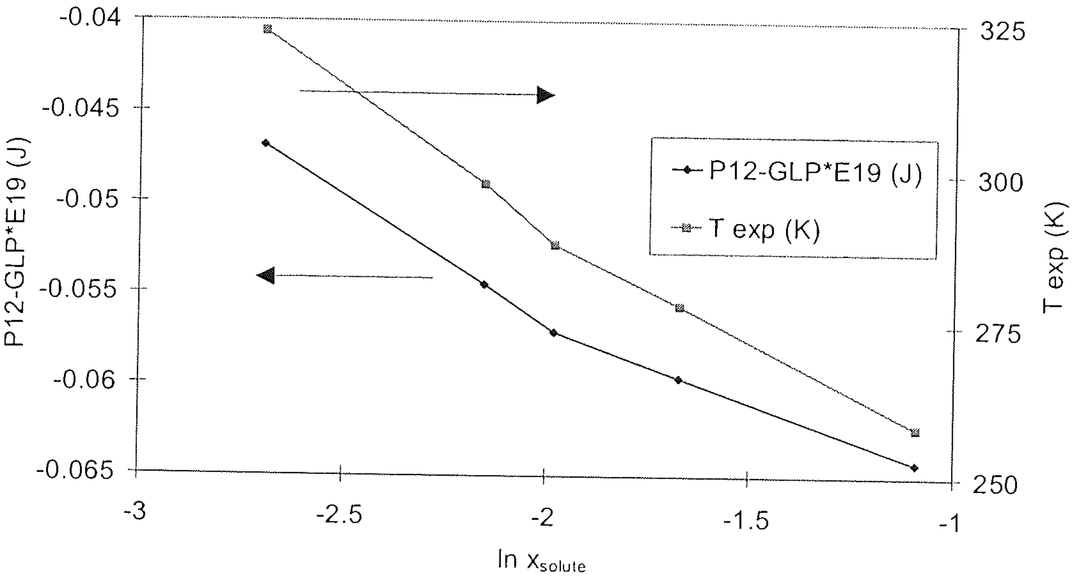

Figure A10.1. Temperature and unlike London pair potentials as a function of the natural logarithm of the solubility for n-propane (1) and n-hexane (2).

mixture solute-solvent	T exp (K)	solubility x_1	ln (x_1)	R^A_1 *E10 (m)	R^A_2*E10 (m)	Φ_{11}*E19 (J)	Φ_{22}*E19 (J)	Φ_{12}-GLP*E19 (J)	Φ_{12}-GM*E19 (J)
n-C_3H_8 + C_6H_6	283.15	0.0813	-2.509609262	5.72896	6.023628	-0.040266	-0.096554	-0.060427	-0.062352573
n-C_3H_8 + C_6H_6	298.2	0.0581	-2.845589615	5.790484	6.036324	-0.036575	-0.0941	-0.056683	-0.058666068
n-C_3H_8 + C_6H_6	323.15	0.037	-3.296837366	5.936968	6.060738	-0.029354	-0.089611	-0.049145	-0.051287828
n-C_3H_8 + C_6H_6	343.15	0.0255	-3.669076827	6.152788	6.082222	-0.021661	-0.085895	-0.0407	-0.043134344
n-C_3H_8 + n-C_6H_{14}	258.15	0.336	-1.090644119	5.649859	6.59498	-0.045728	-0.095345	-0.064205	-0.066029813
n-C_3H_8 + n-C_6H_{14}	278.15	0.188	-1.671313316	5.711382	6.617441	-0.041405	-0.091667	-0.059572	-0.061607403
n-C_3H_8 + n-C_6H_{14}	288.2	0.138	-1.980501594	5.747515	6.630136	-0.039105	-0.08965	-0.057082	-0.059209486
n-C_3H_8 + n-C_6H_{14}	298.2	0.116	-2.154165088	5.790484	6.641855	-0.036575	-0.08782	-0.054457	-0.056674655
n-C_3H_8 + n-C_6H_{14}	323.15	0.0675	-2.695627681	5.936968	6.676035	-0.029354	-0.08269	-0.046848	-0.049267456
n-C_3H_8 + c-C_6H_{12}	283.15	0.136	-1.995100393	5.72896	6.308433	-0.04027	-0.094419	-0.060815	-0.061662413
n-C_3H_8 + c-C_6H_{12}	298.2	0.0924	-2.3816283	5.790484	6.325035	-0.03658	-0.091765	-0.057076	-0.057937585
n-C_3H_8 + c-C_6H_{12}	323.15	0.0555	-2.891372258	5.936968	6.354331	-0.02935	-0.087315	-0.049683	-0.05062307
n-C_3H_8 + c-C_6H_{12}	343.15	0.0371	-3.294138309	6.152788	6.379722	-0.02166	-0.083686	-0.041413	-0.042575096
n-C_3H_8 + CCl_4	258.15	0.254	-1.370421012	5.649859	5.87396	-0.04573	-0.097658	-0.066613	-0.066827392
n-C_3H_8 + CCl_4	273.15	0.155	-1.864330162	5.694781	5.890562	-0.04252	-0.095236	-0.063489	-0.063635169
n-C_3H_8 + CCl_4	298.2	0.0813	-2.509609262	5.790484	5.920835	-0.03658	-0.091008	-0.057642	-0.057698116
n-C_3H_8 + CCl_4	323.15	0.0497	-3.001750346	5.936968	5.953062	-0.02935	-0.086759	-0.050449	-0.050461635
n-C_3H_8 + CS_2	258.15	0.146	-1.924148657	5.649859	5.326577	-0.04573	-0.081692	-0.06054	-0.061120988
n-C_3H_8 + CS_2	273.15	0.0842	-2.474560358	5.694781	5.344156	-0.04252	-0.079553	-0.057661	-0.058160068
n-C_3H_8 + CS_2	298.15	0.0446	-3.11002142	5.789507	5.375406	-0.03663	-0.075917	-0.052358	-0.052733668
n-C_3H_8 + CS_2	308.15	0.0345	-3.366795955	5.840288	5.389077	-0.03389	-0.07439	-0.049879	-0.050210329
n-C_3H_8 + CH_3OH	298.2	0.0115	-4.465408244	5.790484	4.10301	-0.036575	-0.10761	-0.05541	-0.06273624
n-C_3H_8 + C_2H_5OH	298.2	0.0228	-3.780994743	5.790484	5.052092	-0.036575	-0.12275	-0.057434	-0.067004338

Table A10-1. The results of calculations of pair of potentials for a number of mixtures at different temperatures (continued over).

mixture solute-solvent	T exp (K)	solubility x_1	ln (x_1)	R^A_1 *E10 (m)	R^A_2*E10 (m)	Φ_{11}*E19 (J)	Φ_{22}*E19 (J)	Φ_{12}-GLP*E19 (J)	Φ_{12}-GM*E19 (J)
n-C_4H_{10} + CCl_4	298.2	0.339	-1.081755172	6.146469	5.920835	-0.05563	-0.091008	-0.07026	-0.07115318
n-C_4H_{10} + CCl_4	323.15	0.167	-1.789761467	6.211899	5.953062	-0.0499	-0.086759	-0.065129	-0.06579722
n-C_4H_{10} + n-C_6H_{14}	278.15	0.737	-0.305167387	6.105453	6.617441	-0.05967	-0.091667	-0.07406	-0.073957893
n-C_4H_{10} + n-C_6H_{14}	288.2	0.441	-0.818710404	6.124985	6.630136	-0.0577	-0.089647	-0.071872	-0.071921012
n-C_4H_{10} + n-C_6H_{14}	298.2	0.386	-0.95191791	6.146469	6.641855	-0.05563	-0.087819	-0.069706	-0.069895429
n-C_4H_{10} + n-C_6H_{14}	323.15	0.199	-1.614450454	6.211899	6.676035	-0.0499	-0.082692	-0.06371	-0.064236522
n-C_4H_{10} + CH_3OH	298.2	0.0398	-3.223888367	6.146469	4.10301	-0.05563	-0.107612	-0.06912	-0.077372189
n-C_4H_{10} + C_2H_5OH	298.2	0.0815	-2.507152259	6.146469	5.052092	-0.05563	-0.122746	-0.074106	-0.082633891
CO_2 + n-C_6H_{14}	293.2	0.0126	-4.374058465	4.713138	6.635996	-0.0142	-0.088729	-0.029314	-0.0354958
CO_2 + n-C_6H_{14}	298.2	0.0119	-4.431216879	4.994388	6.641855	-0.00959	-0.087819	-0.023656	-0.02902041
CO_2 + n-C_6H_{14}	303.2	0.0113	-4.482952553	7.421145	6.648691	-0.00075	-0.086769	-0.005511	-0.008067016
CO_2 + c-C_6H_{12}	298.2	0.00759	-4.880923688	4.994388	6.325035	-0.00959	-0.091765	-0.025647	-0.029665238
CO_2 + C_6H_6	298.2	0.00912	-4.697285475	4.994388	6.036324	-0.00959	-0.0941	-0.025333	-0.03004029
CO_2 + CH_3OH	298.2	0.00643	-5.046780741	4.994388	4.10301	-0.00959	-0.107612	-0.025901	-0.032124742
CO_2 + C_2H_5OH	298.2	0.00728	-4.922624417	4.994388	5.052092	-0.00959	-0.122746	-0.02494	-0.034309389
CO_2 + CS_2	281.65	0.003785	-5.576709392	4.444583	5.353921	-0.02131	-0.078394	-0.03996	-0.040872682
CO_2 + CS_2	289.7	0.003538	-5.644193683	4.602786	5.363687	-0.01671	-0.077256	-0.035199	-0.035929761
CO_2 + CS_2	298.15	0.00328	-5.719911857	4.989505	5.375406	-0.00965	-0.075917	-0.026399	-0.027066567

Table A10-1. The results of calculations of pair of potentials for a number of mixtures at different temperatures.

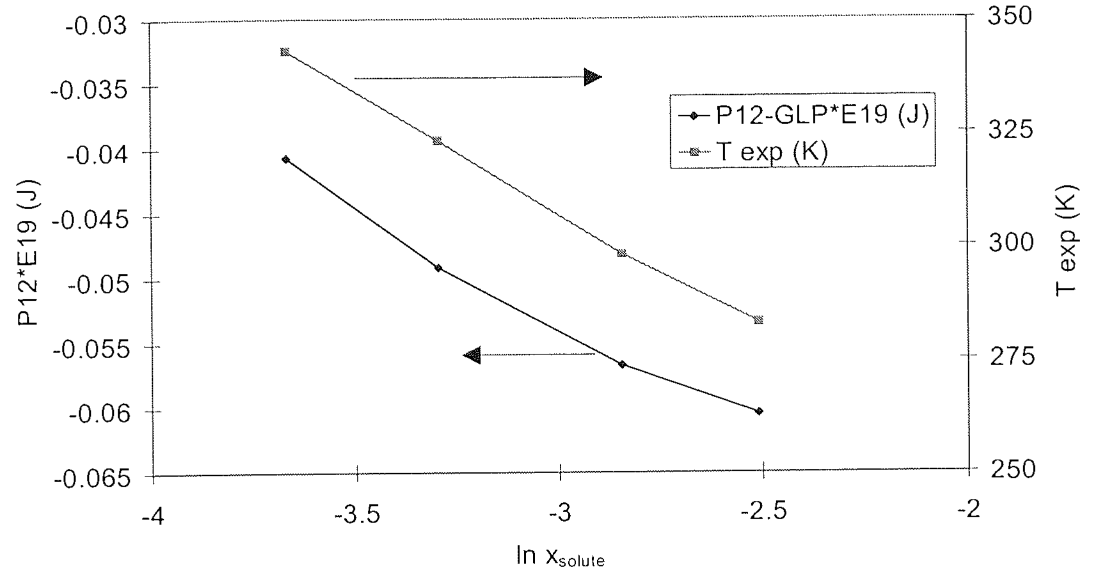

Figure A10.2. Temperature and unlike London pair potentials as a function of the natural logarithm of the solubility for n-propane (1) and benzene (2).

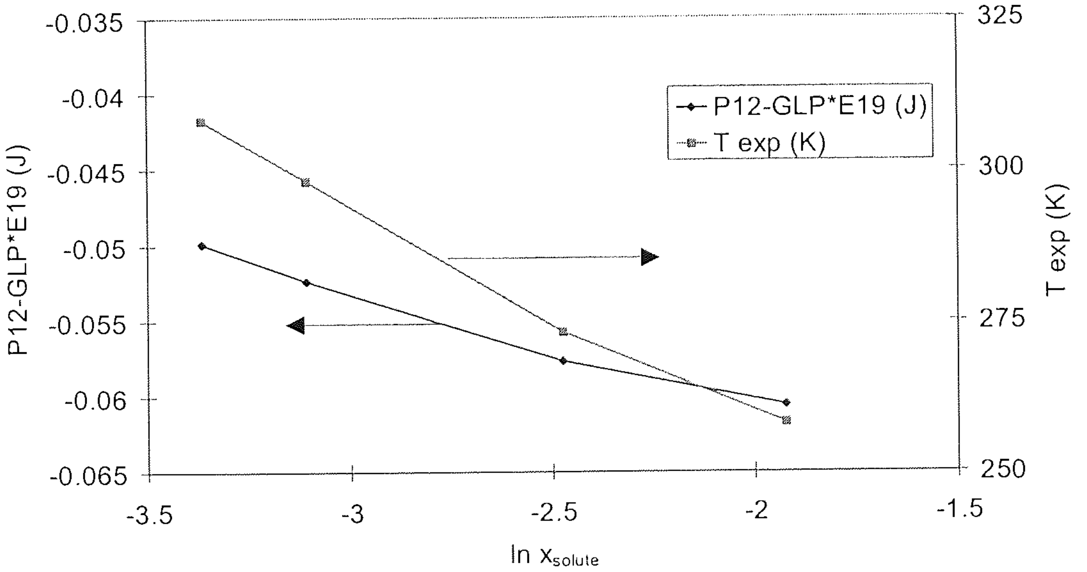

Figure A10.3. Temperature and unlike London pair potentials as a function of the natural logarithm of the solubility for n-propane (1) and carbon disulphide (2).

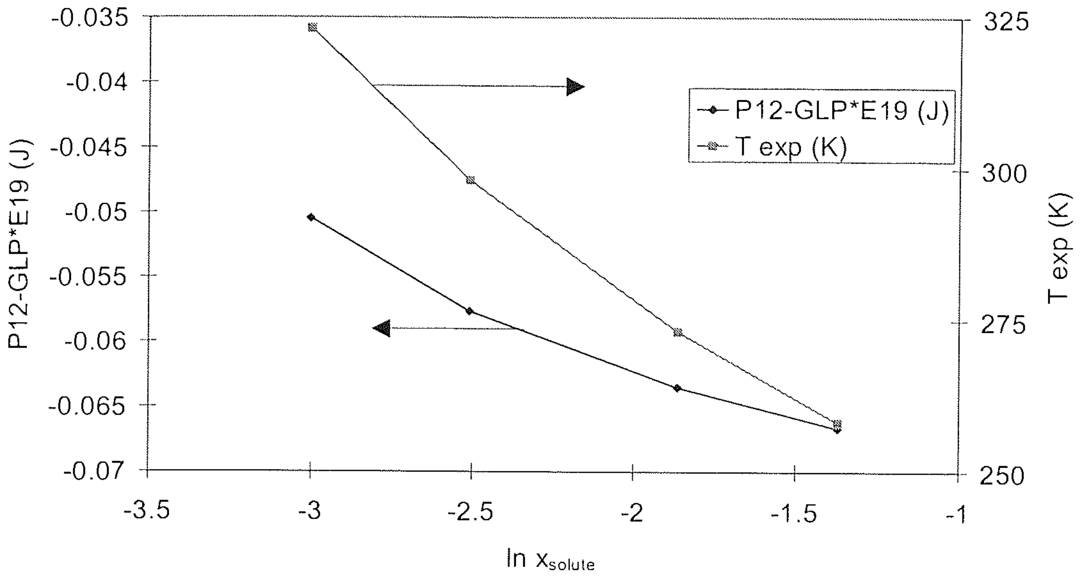

Figure A10.4. Temperature and unlike London pair potentials as a function of the natural logarithm of the solubility for n-propane (1) and carbon tetrachloride (2).

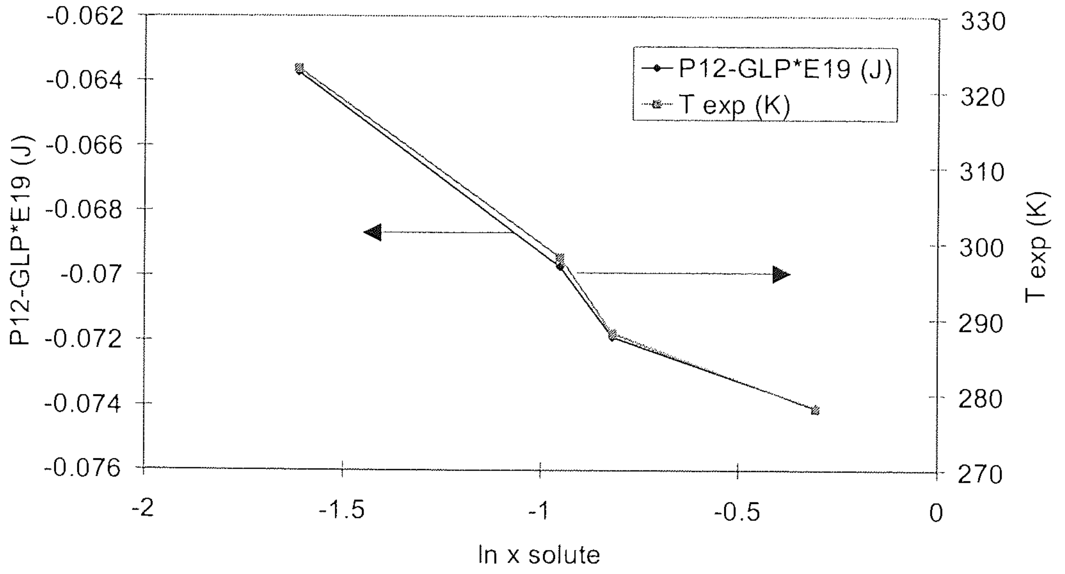

Figure A10.5. Temperature and unlike London pair potentials as a function of the natural logarithm of the solubility for n-butane (1) and n-hexane (2).

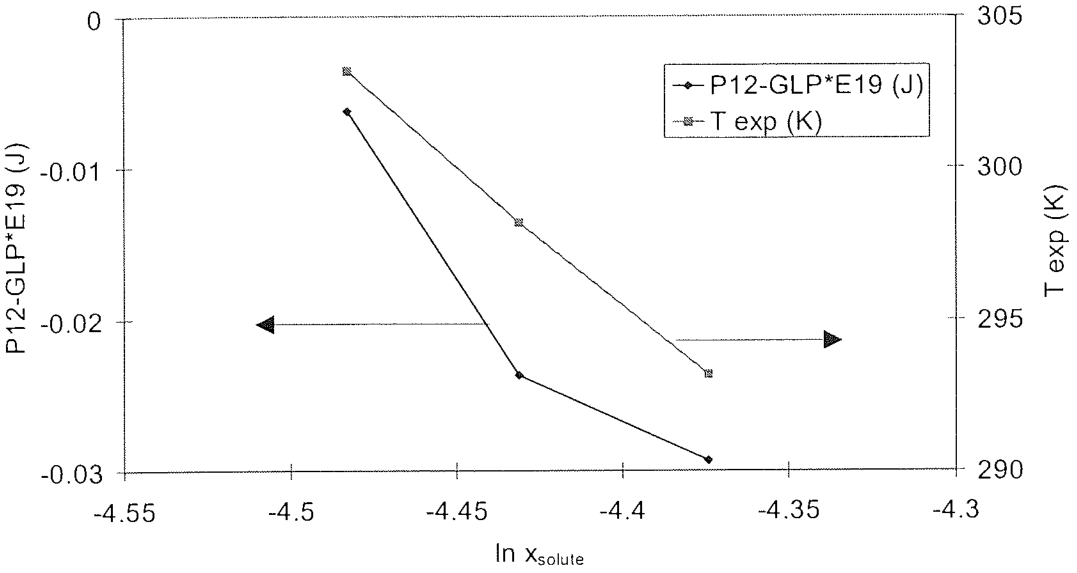

Figure A10.6. Temperature and unlike London pair potentials as a function of the natural logarithm of the solubility for carbon dioxide (1) and n-hexane (2).

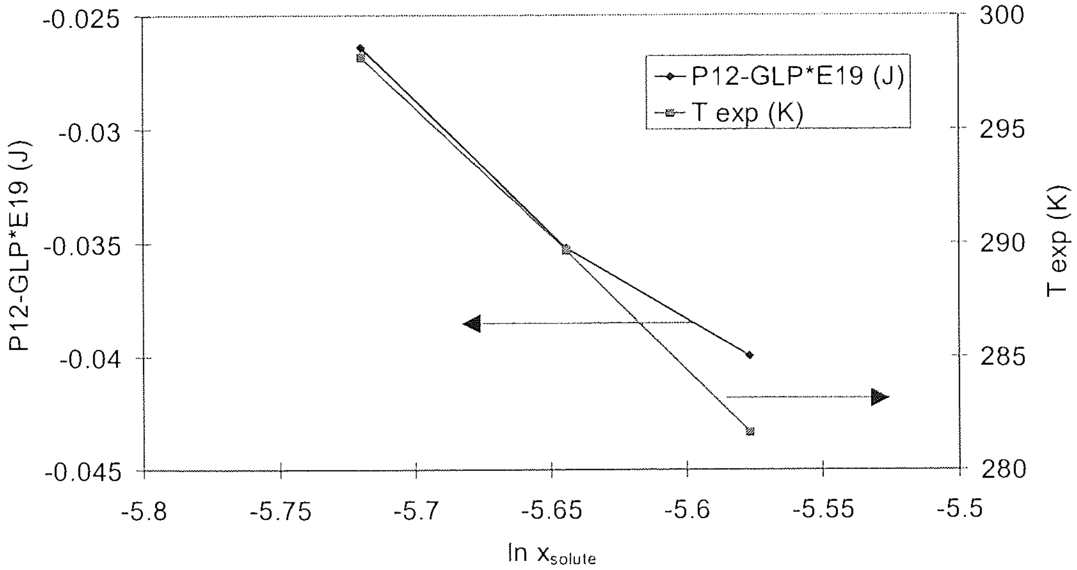

Figure A10.7. Temperature and unlike London pair potentials as a function of the natural logarithm of the solubility for carbon dioxide (1) and carbon disulphide (2).

Appendix 11 - Results of prediction of solubilities using three different methods

A11.1 Results of prediction of solubilities using three different lattice methods

Table A11-1 shows the chosen mixtures (column 1), and which methods can be employed to predict solubilities (columns 2, 3, and 4). All the mentioned methods are available as executable programs.

mixture/method	exp. data	AGAPE	UNIFAC MHV2	UNIFAC ref. sol-vent
$C_3H_8 + C_6H_6$	yes	yes	yes	no
C_3H_8 + n-C_6H_{14}	yes	yes	yes	no
C_3H_8 + c-C_6H_{12}	yes	yes	no	no
$C_3H_8 + CCl_4$	yes	yes	no	no
$C_3H_8 + CS_2$	yes	yes	no	no
$C_3H_8 + CH_3OH$	yes	yes	yes	no
$C_3H_8 + C_2H_5OH$	yes	yes	yes	no
n-C_4H_{10} + CCl_4	yes	yes	no	no
n-C_4H_{10} + n-C_6H_{14}	yes	yes	yes	no
n-C_4H_{10} + CH_3OH	yes	yes	yes	no
n-C_4H_{10} + C_2H_5OH	yes	yes	yes	no
CO_2 + n-C_6H_{14}	yes	yes	yes	yes
CO_2 + c-C_6H_{12}	yes	yes	no	yes
$CO_2 + C_6H_6$	yes	yes	yes	yes
$CO_2 + CH_3OH$	yes	yes	yes	yes
$CO_2 + C_2H_5OH$	yes	yes	yes	yes
$CO_2 + CS_2$	yes	yes	no	no

Table A11-1. The chosen mixtures and which methods can be employed to predict solubilities.

The results obtained of the performed calculations are shown in Tables A11-2, A11-3, A11-4, and A11-5. Tables A11-2, A11-3, and A11-4 have similar features, Table A11-2 shows the results of isothermal AGAPE calculations, Table A11-3 shows the results of isobaric AGAPE calculations, and Table A11-4 shows the results of isothermal MHV2 calculations. Table A11-5 displays the results of the reference solvent calculations.

In Tables A11-2, A11-3, A11-4, and A11-5 the first column shows the mixture, the solute's name first, then follows the experimental data in columns 2 to 4. The experimental data are from Fogg and Gerrard (1991) or IUPAC Solubility Data Series, Hayduk, 1986 (vol. 24). The solubility (liquid mole fraction of the solute (component 1)) is in column two, then the temperature and then the total pressure, which is assumed to be equal to the partial pressure of the solute (assumption discussed in section 4.6). The fifth and the sixth columns again show experimental data. These data are calculated assuming the activity coefficient (γ_2) of the solvent (component 2) is equal to unity. This assumption is also discussed in section 4.6. Equation (4.15) is then used to give an estimated value of the vapour phase mole fraction of the solute (y_1) and the activity coefficient of the solute (γ_1) is calculated using equation (4.18). These estimated values give more results with which to compare the predicted results. The experimental solubility measurements contain no information of a measurement of the vapour phase composition and it was therefore necessary to estimated the vapour composition.

Then follow the predicted results in the next columns. In Table A11-2 and Table A11-4 the seventh column shows the predicted total pressure. The seventh column in Table A11-3 shows the predicted temperature. Then follow, for the three tables mentioned, the predicted mole fraction of the solute (component 1) and the activity coefficients, first for the solute, then for the solvent. The last three columns are the calculated errors in %. The errors are calculated as

$$\Delta = (\text{predicted} - \text{experimental}) * 100 / \text{experimental} \qquad (\text{A11.1})$$

This equation is used to calculate the ΔP, Δy_1, and $\Delta \gamma_1$ which are displayed in the last three columns.

Table A11-5 contains rather more information then the three first tables. This is because the reference solvent method calculates the solubility from the input pressure and temperature as opposed to the two methods mentioned above, where temperature, pressure and solubility are the input data. Columns 1 to 6 show the same data as the three other tables. Then follows the predicted results with the solubility in column 7, the vapour phase mole fraction of the solute in column 8 and the activity coefficients for the solute and the solvent in columns 9 and 10, respectively.

Again, the last four columns display the errors as calculated by equation (A11.1), Δx_1, ΔP, Δy_1, and $\Delta \gamma_1$, which are displayed in the last four columns.

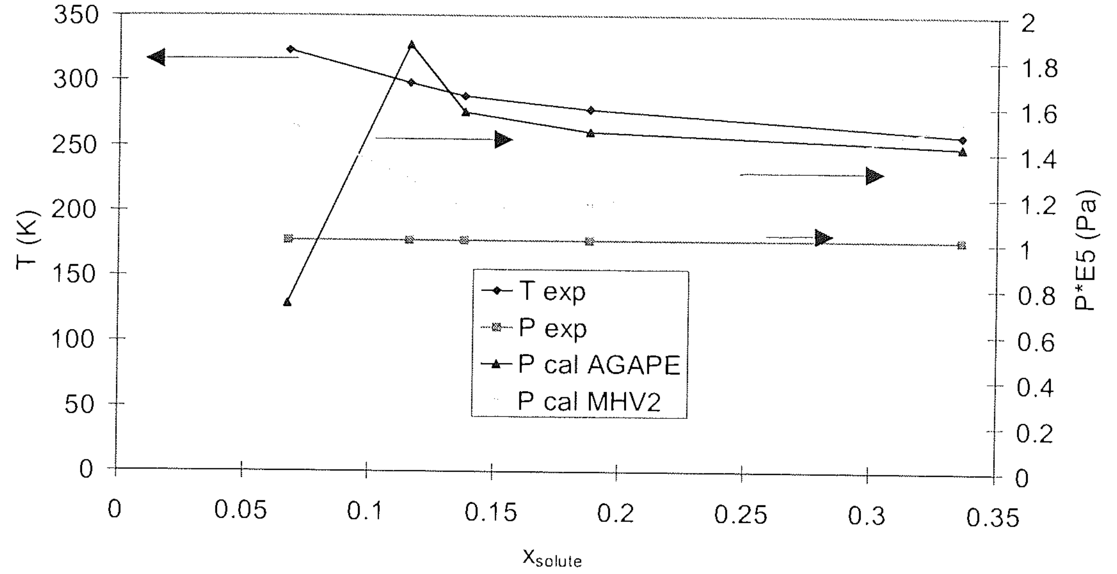

Figure A11.1 The experimental temperature (left y-axis) and experimental pressure and pressures predicted by the AGAPE and MHV2 methods (right y-axis) as a function of the solubility for n-propane (1) and n-hexane (2).

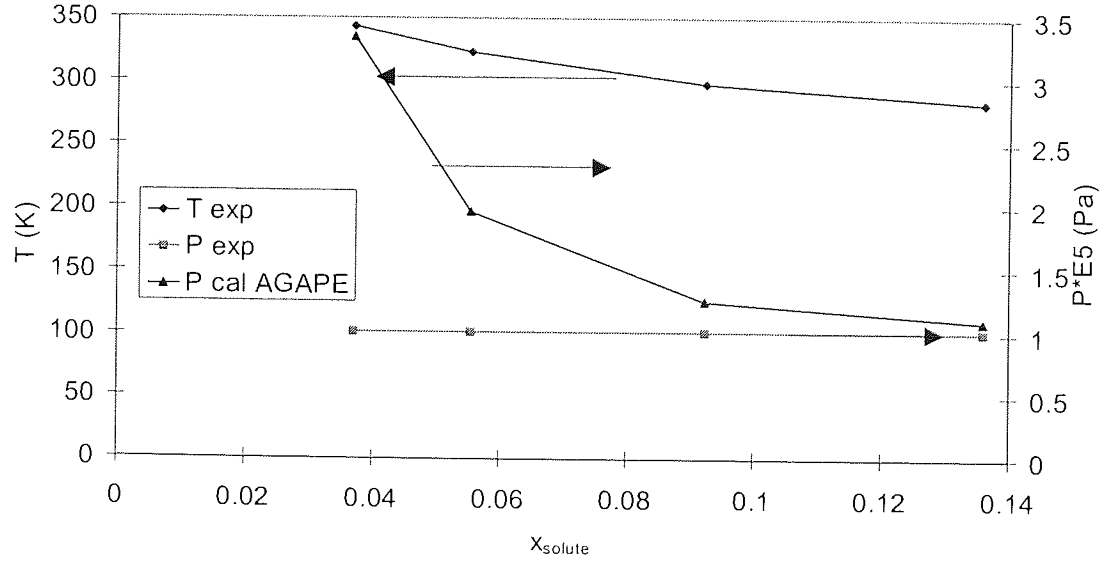

Figure A11.2. The experimental temperature (left y-axis) and experimental pressure and pressures predicted by the AGAPE method (right y-axis) as a function of the solubility for n-propane (1) and *cyclo*-hexane (2).

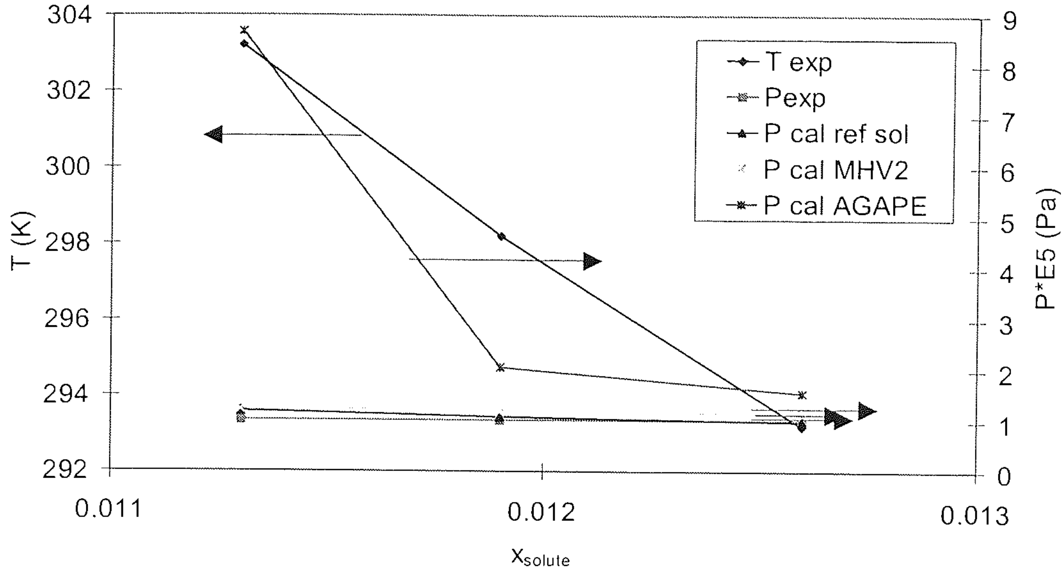

Figure A11.3. The experimental temperature (left y-axis) and experimental pressure and pressures predicted by the AGAPE, MHV2 and reference solvent methods (right y-axis) as a function of the solubility for carbon dioxide (1) and n-hexane (2).

Method	Experimental			Calculated from experimental data assuming $\gamma_2 = 1.0$		AGAPE isobaric				ERRORS AGAPE isobaric	% AGAPE- "y"exp	% AGAPE- "y"exp
Mixture	x_1	T exp (K)	P exp (10^5 Pa)	y_1	γ_1	T cal (K) AGAPE	y_1	γ_1	γ_2	ΔT	Δy	$\Delta \gamma_1$
$C_3H_8 + C_6H_6$	0.0813	283.15	1.013	0.9455	1.8696	289.52	0.9251	1.5367	1.0013	2.25	2.16	46.44
$C_3H_8 + C_6H_6$	0.0581	298.2	1.013	0.8831	1.6576	298.74	0.88	1.6073	1.0007	0.18	0.35	39.63
$C_3H_8 + C_6H_6$	0.037	323.15	1.013	0.6603	1.0687	310.39	0.7966	1.7199	1.0003	3.95	20.65	6.40
$C_3H_8 + C_6H_6$	0.0255	343.15	1.013	0.3023	0.4703	318.93	0.708	1.825	1.0002	7.06	134.17	112.67
$C_3H_8 + n\text{-}C_6H_{14}$	0.336	258.15	1.013	0.6295	0.6583	253.85	0.9873	1.2013	1.0245	1.67	56.85	55.62
$C_3H_8 + n\text{-}C_6H_{14}$	0.188	278.15	1.013	0.9370	0.9254	269.41	0.9605	1.2393	1.0056	3.14	2.51	8.67
$C_3H_8 + n\text{-}C_6H_{14}$	0.138	288.2	1.013	0.8907	0.9031	278.41	0.9324	1.2467	1.0027	3.40	4.69	11.03
$C_3H_8 + n\text{-}C_6H_{14}$	0.116	298.2	1.013	0.8237	0.7637	283.54	0.9107	1.2502	1.0018	4.92	10.57	31.17
$C_3H_8 + n\text{-}C_6H_{14}$	0.0675	323.15	1.013	0.8661	2.8536	299.04	0.808	1.2608	1.0005	7.46	6.71	64.94
$C_3H_8 + c\text{-}C_6H_{12}$	0.136	283.15	1.013	0.9463	1.1203	283.34	0.9459	1.1141	1.0008	0.07	0.05	10.66
$C_3H_8 + c\text{-}C_6H_{12}$	0.0924	298.2	1.013	0.8839	1.0447	295.15	0.8995	1.1314	1.0003	1.02	1.76	4.25
$C_3H_8 + c\text{-}C_6H_{12}$	0.0555	323.15	1.013	0.6650	0.7175	309.78	0.8015	1.1705	1.0001	4.14	20.52	39.38
$C_3H_8 + c\text{-}C_6H_{12}$	0.0371	343.15	1.013	0.3168	0.3388	319.78	0.7001	1.2173	1.0001	6.81	120.98	195.23
$C_3H_8 + CCl_4$	0.254	258.15	1.013	0.9865	1.3648	267.7	0.9763	1.0204	0.9977	3.70	1.04	26.90
$C_3H_8 + CCl_4$	0.155	273.15	1.013	0.9634	1.3424	281.33	0.9441	1.0332	0.9992	2.99	2.00	25.57
$C_3H_8 + CCl_4$	0.0813	298.2	1.013	0.8632	1.1419	300.08	0.8512	1.074	0.9999	0.63	1.39	12.44
$C_3H_8 + CCl_4$	0.0497	323.15	1.013	0.7590	1.4667	312.76	0.7398	1.1253	1	3.22	2.53	31.82
$C_3H_8 + CS_2$	0.146	258.15	1.013	0.9330	2.2456	270.96	0.8715	1.3794	1.0056	4.96	6.60	55.22
$C_3H_8 + CS_2$	0.0842	273.15	1.013	0.8492	2.1782	282.78	0.7672	1.4829	1.0021	3.53	9.65	53.99
$C_3H_8 + CS_2$	0.0446	298.15	1.013	0.5511	1.3290	294.78	0.607	1.599	1.0007	1.13	10.14	24.71
$C_3H_8 + CS_2$	0.0345	308.15	1.013	0.3479	0.8492	298.84	0.5355	1.6431	1.0004	3.02	53.93	17.80
$C_3H_8 + CH_3OH$	0.02039	273.2	1.0084	0.9605	10.1288	289.91	0.8932	5.8252	0.9996	6.12	7.01	90.13
$C_3H_8 + CH_3OH$	0.004988	298.2	0.6186	0.7263	9.5646	301.23	0.6803	8.3016	1	1.02	6.34	89.54
$C_3H_8 + CH_3OH$	0.00704	298.2	0.7974	0.7883	9.4791	301.35	0.7522	8.357	1	1.06	4.57	89.45
$C_3H_8 + CH_3OH$	0.009569	298.2	1.0127	0.8337	9.3674	301.29	0.8042	8.3618	1	1.04	3.53	89.32
$C_3H_8 + CH_3OH$	0.0115	298.2	1.013	0.8339	7.7997	298.66	0.8309	7.6809	0.9999	0.15	0.36	87.18

Table A11-2. Results of computer calculations using the AGAPE method, isobaric case (continued over).

Method	Experimental			Calculated from experimental data assuming γ_2 = 1.0		AGAPE isobaric				ERRORS AGAPE isobaric	% AGAPE-"y"exp	% AGAPE-"y"exp
Mixture	x_1	T exp (K)	P exp (10^5 Pa)	y_1	γ_1	T cal (K) AGAPE	y_1	γ_1	γ_2	Δ T	Δ y	Δ γ_1
C_3H_8 + CH_3OH	0.003232	323.2	1.0111	0.4503	8.3185							
C_3H_8 + C_2H_5OH	0.01497	273.2	0.413	0.9616	5.6562	281.23	0.935	4.3307	0.9999	2.94	2.77	82.32
C_3H_8 + C_2H_5OH	0.02706	273.2	0.7093	0.9779	5.4649	280.73	0.962	4.2947	0.9998	2.76	1.63	81.71
C_3H_8 + C_2H_5OH	0.04054	273.2	1.016	0.9848	5.2622	279.98	0.9752	4.254	0.9996	2.48	0.98	81.00
C_3H_8 + C_2H_5OH	0.005089	298.2	0.331	0.7628	5.2753	295.35	0.7984	5.9322	1	0.96	4.66	81.04
C_3H_8 + C_2H_5OH	0.01003	298.2	0.5699	0.8629	5.2126	294.79	0.8886	5.8527	1	1.14	2.98	80.82
C_3H_8 + C_2H_5OH	0.01434	298.2	0.773	0.8994	5.1542	294.43	0.9178	5.7887	1	1.26	2.05	80.60
C_3H_8 + C_2H_5OH	0.01941	298.2	1.007	0.9232	5.0919	294.1	0.9396	5.7525	1	1.37	1.77	80.36
C_3H_8 + C_2H_5OH	0.0228	298.2	1.013	0.9237	4.3573	291.1	0.9502	5.3932	1.9	2.38	2.87	56.40
C_3H_8 + C_2H_5OH	0.003201	323.15	0.5493	0.4643	4.7095	312.85	0.6801	8.6893	1	3.19	46.49	78.77
C_3H_8 + C_2H_5OH	0.006342	323.15	0.7951	0.6309	4.6762	309.87	0.8105	8.111	1	4.11	28.46	78.61
C_3H_8 + C_2H_5OH	0.009245	323.15	1.0191	0.7129	4.6455	308.47	0.8631	7.8498	1	4.54	21.07	78.47
n-C_4H_{10} + CCl_4	0.339	298.2	1.013	0.9016	1.1026	297.26	0.9047	1.1392	1.0187	0.32	0.34	7.61
n-C_4H_{10} + CCl_4	0.167	323.15	1.013	0.6613	0.8069	314.14	0.7593	1.1809	1.0036	2.79	14.82	24.37
n-C_4H_{10} + n-C_6H_{14}	0.737	278.15	1.013	0.9796	1.0805	280.59	0.9785	0.9887	0.9596	0.88	0.11	11.19
n-C_4H_{10} + n-C_6H_{14}	0.441	288.2	1.013	0.9291	1.2061	293.78	0.908	0.9817	0.9952	1.94	2.27	17.49
n-C_4H_{10} + n-C_6H_{14}	0.386	298.2	1.013	0.8776	0.9426	297.09	0.8841	0.9831	0.9973	0.37	0.75	5.80
n-C_4H_{10} + n-C_6H_{14}	0.199	323.15	1.013	0.5729	0.5867	311.9	0.7202	1.0005	1.0002	3.48	25.70	70.49
n-C_4H_{10} + CH_3OH	0.01651	298.2	0.6594	0.7462	12.1981	310.64	0.5296	5.9827	0.9996	4.17	29.03	91.81
n-C_4H_{10} + CH_3OH	0.0241	298.2	0.8474	0.8041	11.5703	311.14	0.6279	6.1566	0.9992	4.34	21.91	91.36
n-C_4H_{10} + CH_3OH	0.0398	298.2	1.013	0.8387	8.7369	307.39	0.7453	5.8903	0.9977	3.08	11.14	88.58
n-C_4H_{10} + CH_3OH	0.03171	298.2	1.0159	0.8378	10.9869	310.95	0.6959	6.2495	0.9987	4.28	16.94	90.91
n-C_4H_{10} + CH_3OH	0.0192	308.2	1.0007	0.7249	11.4582	317.51	0.5756	7.0113	0.9996	3.02	20.60	91.28
n-C_4H_{10} + CH_3OH	0.008075	323.2	1.009	0.4518	11.3405	326.64	0.3649	8.3826	1	1.06	19.23	91.18
n-C_4H_{10} + C_2H_5OH	0.01517	298.2	0.3173	0.7551	6.4731	307.53	0.5888	3.8089	0.9999	3.13	22.02	84.55
n-C_4H_{10} + C_2H_5OH	0.02334	298.2	0.4344	0.8227	6.2771	308.21	0.6894	3.8898	0.9997	3.36	16.20	84.07

Table A11-2. Results of computer calculations using the AGAPE method, isobaric case (continued over).

Method	Experimental			Calculated from experimental data assuming $\gamma_2 = 1.0$		AGAPE isobaric				ERRORS AGAPE isobaric	% AGAPE-"y"exp	% AGAPE-"y"exp
Mixture	x_1	T exp (K)	P exp (10^5 Pa)	y_1	γ_1	T cal (K) AGAPE	y_1	γ_1	γ_2	Δ T	Δ y	$\Delta \gamma_1$
n-C_4H_{10} + C_2H_5OH	0.02999	298.2	0.5244	0.8540	6.1209	308.28	0.7423	3.928	0.9995	3.38	13.08	83.67
n-C_4H_{10} + C_2H_5OH	0.0344	298.2	0.5824	0.8692	6.0329	308.28	0.7696	3.943	0.9994	3.38	11.46	83.43
n-C_4H_{10} + C_2H_5OH	0.05144	298.2	0.7865	0.9048	5.6711	307.65	0.8382	9.9492	0.9988	3.17	7.37	82.39
n-C_4H_{10} + C_2H_5OH	0.07092	298.2	0.9859	0.9257	5.2747	306.53	0.8821	3.9175	0.9979	2.79	4.71	81.08
n-C_4H_{10} + C_2H_5OH	0.0815	298.2	1.013	0.9282	4.7222	304.28	0.8982	3.7989	0.997	2.04	3.24	78.89
n-C_4H_{10} + C_2H_5OH	0.008298	308.2	0.3106	0.5592	6.3486	313.15	0.4273	4.2149	1	1.61	23.59	84.25
n-C_4H_{10} + C_2H_5OH	0.01484	308.2	0.4401	0.6917	6.2307	314.28	0.573	4.3397	0.9999	1.97	17.17	83.95
n-C_4H_{10} + C_2H_5OH	0.02198	308.2	0.574	0.7654	6.0705	314.78	0.6675	4.3907	0.9998	2.13	12.79	83.53
n-C_4H_{10} + C_2H_5OH	0.04476	308.2	0.959	0.8628	5.6151	314.43	0.8095	4.4103	0.9995	2.02	6.18	82.20
n-C_4H_{10} + C_2H_5OH	0.00521	323.1	0.4504	0.3479	6.0501	324.4	0.308	5.1854	1	0.40	11.46	83.47
n-C_4H_{10} + C_2H_5OH	0.01218	323.1	0.6499	0.5513	5.9162	324.96	0.5119	5.2417	1	0.58	7.14	83.10
n-C_4H_{10} + C_2H_5OH	0.01716	323.1	0.7874	0.6314	5.8287	325.03	0.5964	5.2439	1	0.60	5.55	82.84
n-C_4H_{10} + C_2H_5OH	0.02442	323.1	0.9779	0.7055	5.6825	324.93	0.6789	5.2217	1	0.57	3.77	82.40

Table A11-2. Results of computer calculations using the AGAPE method, isobaric case.

Method	Experimental			Calculated from experimental data assuming γ_2 = 1.0		AGAPE isothermal				ERRORS AGAPE isothermal	% AGAPE- "y"exp	% AGAPE- "y"exp
Mixture	x_1	T exp (K)	P exp (10^5 Pa)	y_1	γ_1	P cal AGAPE (10^5 Pa)	y_1	γ_1	γ_2	Δ P	Δ y	$\Delta \gamma_1$
C_3H_8 + C_6H_6	0.0813	283.15	1.013	0.9455	1.8696	0.8674	0.9363	1.5853	1.0009	14.37	0.97	15.21
C_3H_8 + C_6H_6	0.0581	298.2	1.013	0.8831	1.6576	1.0991	0.8922	1.817	1.0007	8.50	1.03	9.62
C_3H_8 + C_6H_6	0.037	323.15	1.013	0.6603	1.0687	1.9734	0.8255	2.6029	1.0006	94.81	25.03	143.56
C_3H_8 + C_6H_6	0.0255	343.15	1.013	0.3023	0.4703	3.7876	0.8133	4.7302	1.0006	273.90	168.99	905.77
C_3H_8 + n-C_6H_{14}	0.336	258.15	1.013	0.6295	0.6583	1.4251	0.7328	1.0782	1.0145	40.68	16.41	63.77
C_3H_8 + n-C_6H_{14}	0.188	278.15	1.013	0.9370	0.9254	1.491	0.9568	1.3909	1.0086	47.19	2.12	50.30
C_3H_8 + n-C_6H_{14}	0.138	288.2	1.013	0.8907	0.9031	1.5762	0.9294	1.4663	1.0047	55.60	4.35	62.36
C_3H_8 + n-C_6H_{14}	0.116	298.2	1.013	0.8237	0.7637	1.8712	0.9042	1.5487	1.0036	84.72	9.78	102.78
C_3H_8 + n-C_6H_{14}	0.0675	323.15	1.013	0.8661	2.8536	0.737	0.8157	1.9552	1.0017	27.25	5.82	31.48
C_3H_8 + c-C_6H_{12}	0.136	283.15	1.013	0.9463	1.1203	1.0974	0.9504	1.2188	1.0013	8.33	0.43	8.80
C_3H_8 + c-C_6H_{12}	0.0924	298.2	1.013	0.8839	1.0447	1.2586	0.9065	1.3311	1.0009	24.24	2.55	27.42
C_3H_8 + c-C_6H_{12}	0.0555	323.15	1.013	0.6650	0.7175	1.9676	0.8274	1.734	1.0008	94.23	24.42	141.66
C_3H_8 + c-C_6H_{12}	0.0371	343.15	1.013	0.3168	0.3388	3.3476	0.7931	2.8024	1.0008	230.46	150.33	727.26
C_3H_8 + CCl_4	0.254	258.15	1.013	0.9865	1.3648	0.7862	0.9827	1.0551	0.9969	22.39	0.39	22.69
C_3H_8 + CCl_4	0.155	273.15	1.013	0.9634	1.3424	0.8468	0.9562	1.1138	0.9997	16.41	0.74	17.03
C_3H_8 + CCl_4	0.0813	298.2	1.013	0.8632	1.1419	1.1443	0.8788	1.3133	1.0006	12.96	1.81	15.01
C_3H_8 + CCl_4	0.0497	323.15	1.013	0.7590	1.4667	1.1928	0.7952	1.8093	1.0007	17.75	4.77	23.36
C_3H_8 + CS_2	0.146	258.15	1.013	0.9330	2.2456	0.5832	0.8838	1.2246	0.9991	42.43	5.28	45.47
C_3H_8 + CS_2	0.0842	273.15	1.013	0.8492	2.1782	0.6857	0.7771	1.3493	1.0003	32.31	8.49	38.05
C_3H_8 + CS_2	0.0446	298.15	1.013	0.5511	1.3290	1.1709	0.6114	1.7043	1.0006	15.59	10.94	28.24
C_3H_8 + CS_2	0.0345	308.15	1.013	0.3479	0.8492	1.4687	0.55	1.9465	1.0005	44.99	58.09	129.21
C_3H_8 + CH_3OH	0.02039	273.2	1.0084	0.9605	10.1288	0.4018	0.901	3.7858	0.9989	60.15	6.20	62.62
C_3H_8 + CH_3OH	0.004988	298.2	0.6186	0.7263	9.5646	0.7158	0.7635	11.6337	1	15.71	5.12	21.63
C_3H_8 + CH_3OH	0.00704	298.2	0.7974	0.7883	9.4791	0.9427	0.82089	11.6703	1	18.22	4.14	23.12

Table A11-3. Results of computer calculations using the AGAPE method, isothermal case (continued over).

Method	Experimental			Calculated from experimental data assuming $\gamma_2 = 1.0$		AGAPE isothermal				ERRORS AGAPE isothermal	% AGAPE-"y"exp	% AGAPE-"y"exp
Mixture	x_1	T exp (K)	P exp (10^5 Pa)	y_1	γ_1	P cal AGAPE (10^5 Pa)	y_1	γ_1	γ_2	ΔP	Δy	$\Delta \gamma_1$
$C_3H_8 + CH_3OH$	0.009569	298.2	1.0127	0.8337	9.3674	1.2241	0.8624	11.7132	0.9999	20.87	3.45	25.04
$C_3H_8 + CH_3OH$	0.0115	298.2	1.013	0.8339	7.7997	1.4402	0.8832	11.7441	0.9999	42.17	5.91	50.57
$C_3H_8 + CH_3OH$	0.003232	323.2	1.0111	0.4503	8.3185	3.0861	0.8199	46.23	1	205.22	82.08	455.75
$C_3H_8 + C_2H_5OH$	0.01497	273.2	0.413	0.9616	5.6562	0.2919	0.9457	3.9315	0.9998	29.32	1.65	30.49
$C_3H_8 + C_2H_5OH$	0.02706	273.2	0.7093	0.9779	5.4649	0.5248	0.9702	4.0114	0.9994	26.01	0.79	26.60
$C_3H_8 + C_2H_5OH$	0.04054	273.2	1.016	0.9848	5.2622	0.794	0.9806	4.0948	0.9987	21.85	0.43	22.19
$C_3H_8 + C_2H_5OH$	0.005089	298.2	0.331	0.7628	5.2753	0.5168	0.8481	9.1572	1	56.13	11.18	73.58
$C_3H_8 + C_2H_5OH$	0.01003	298.2	0.5699	0.8629	5.2126	0.9415	0.917	9.1516	1	65.20	6.27	75.57
$C_3H_8 + C_2H_5OH$	0.01434	298.2	0.773	0.8994	5.1542	1.3113	0.9407	9.145	1	69.64	4.59	77.43
$C_3H_8 + C_2H_5OH$	0.01941	298.2	1.007	0.9232	5.0919	1.7452	0.9557	9.1351	1	73.31	3.52	79.40
$C_3H_8 + C_2H_5OH$	0.0228	298.2	1.013	0.9237	4.3573	2.0454	0.9622	9.165	1.0001	101.92	4.17	110.33
$C_3H_8 + C_2H_5OH$	0.003201	323.15	0.5493	0.4643	4.7095	1.6768	0.8245	25.5311	1	205.26	77.59	442.12
$C_3H_8 + C_2H_5OH$	0.006342	323.15	0.7951	0.6309	4.6762	3.0101	0.9025	25.3234	1.0001	278.58	43.05	441.54
$C_3H_8 + C_2H_5OH$	0.009245	323.15	1.0191	0.7129	4.6455	4.2228	0.9307	25.1314	1.0001	314.37	30.56	440.98
$n\text{-}C_4H_{10} + CCl_4$	0.339	298.2	1.013	0.9016	1.1026	1.0673	0.9047	1.1657	1.0205	5.36	0.34	5.72
$n\text{-}C_4H_{10} + CCl_4$	0.167	323.15	1.013	0.6613	0.8069	1.3922	0.7523	1.2616	1.0051	37.43	13.76	56.34
$n\text{-}C_4H_{10} + n\text{-}C_6H_{14}$	0.737	278.15	1.013	0.9796	1.0805	0.9318	0.9785	0.9928	0.9697	8.02	0.11	8.12
$n\text{-}C_4H_{10} + n\text{-}C_6H_{14}$	0.441	288.2	1.013	0.9291	1.2061	0.8464	0.9153	0.9928	0.9977	16.45	1.48	17.68
$n\text{-}C_4H_{10} + n\text{-}C_6H_{14}$	0.386	298.2	1.013	0.8776	0.9426	1.0754	0.8844	1.0085	1.0023	6.16	0.78	6.99
$n\text{-}C_4H_{10} + n\text{-}C_6H_{14}$	0.199	323.15	1.013	0.5729	0.5867	1.4985	0.7105	1.0762	1.0028	47.93	24.01	83.44
$n\text{-}C_4H_{10} + CH_3OH$	0.01651	298.2	0.6594	0.7462	12.1981	0.3751	0.5543	5.1542	0.9991	43.11	25.72	57.75
$n\text{-}C_4H_{10} + CH_3OH$	0.0398	298.2	1.013	0.8387	8.7369	0.7248	0.7755	5.7801	0.9959	28.45	7.54	33.84
$n\text{-}C_4H_{10} + CH_3OH$	0.0241	298.2	0.8474	0.8041	11.5703	0.4822	0.6563	5.3738	0.9983	43.10	18.38	53.56
$n\text{-}C_4H_{10} + CH_3OH$	0.0192	308.2	1.0007	0.7249	11.4582	0.72422	0.6202	7.0946	0.9992	27.63	14.44	38.08
$n\text{-}C_4H_{10} + CH_3OH$	0.03171	298.2	1.0159	0.8378	10.9869	0.5965	0.7246	5.5792	0.9972	41.28	13.52	49.22

Table A11-3. Results of computer calculations using the AGAPE method, isothermal case (continued over).

Method	Experimental			Calculated from experimental data assuming $\gamma_2 = 1.0$		AGAPE isothermal				ERRORS AGAPE isothermal	% AGAPE-"y"exp	% AGAPE-"y"exp
Mixture	x_1	T exp (K)	P exp (10^5 Pa)	y_1	γ_1	P cal AGAPE (10^5 Pa)	y_1	γ_1	γ_2	Δ P	Δ y	Δ γ_1
n-C_4H_{10} + CH_3OH	0.008075	323.2	1.009	0.4518	11.3405	0.9847	0.4383	10.7373	0.9999	2.41	2.98	5.32
n-C_4H_{10} + C_2H_5OH	0.01517	298.2	0.3173	0.7551	6.4731	0.201	0.6135	3.3316	0.9997	36.65	18.75	48.53
n-C_4H_{10} + C_2H_5OH	0.02334	298.2	0.4344	0.8227	6.2771	0.2705	0.7154	3.3991	0.9993	37.73	13.04	45.85
n-C_4H_{10} + C_2H_5OH	0.02999	298.2	0.5244	0.8540	6.1209	0.329	0.7676	3.4515	0.9989	37.26	10.12	43.61
n-C_4H_{10} + C_2H_5OH	0.05144	298.2	0.7865	0.9048	5.6711	0.527	0.8584	3.6049	0.9971	32.99	5.13	36.43
n-C_4H_{10} + C_2H_5OH	0.07092	298.2	0.9859	0.9257	5.2747	0.7169	0.8983	3.7221	0.995	27.28	2.96	29.44
n-C_4H_{10} + C_2H_5OH	0.0815	298.2	1.013	0.9282	4.7222	0.8247	0.9124	3.7788	0.9938	18.59	1.71	19.98
n-C_4H_{10} + C_2H_5OH	0.008298	308.2	0.3106	0.5592	6.3486	0.2535	0.46	4.2621	0.9999	18.38	17.74	32.87
n-C_4H_{10} + C_2H_5OH	0.01484	308.2	0.4401	0.6917	6.2307	0.3461	0.6081	4.3074	0.9998	21.36	12.09	30.87
n-C_4H_{10} + C_2H_5OH	0.02198	308.2	0.574	0.7654	6.0705	0.4499	0.7008	4.3565	0.9996	21.62	8.44	28.23
n-C_4H_{10} + C_2H_5OH	0.04476	308.2	0.959	0.8628	5.6151	0.7928	0.8343	4.4885	0.9986	17.33	3.31	20.06
n-C_4H_{10} + C_2H_5OH	0.00521	323.1	0.4504	0.3479	6.0501	0.4537	0.3526	6.1775	1	0.73	1.36	2.11
n-C_4H_{10} + C_2H_5OH	0.01218	323.1	0.6499	0.5513	5.9162	0.6669	0.5627	6.1969	1	2.62	2.08	4.75
n-C_4H_{10} + C_2H_5OH	0.01716	323.1	0.7874	0.6314	5.8287	0.8197	0.646	6.2077	0.9999	4.10	2.31	6.50
n-C_4H_{10} + C_2H_5OH	0.02442	323.1	0.9779	0.7055	5.6825	1.043	0.7239	6.2189	0.9999	6.66	2.61	9.44
CO_2 + n-C_6H_{14}	0.0126	293.2	1.013	0.8423	1.1786	1.5647	0.8979	1.9406	1	54.46	6.60	64.66
CO_2 + n-C_6H_{14}	0.0119	298.2	1.013	0.8030	1.0594	2.0575	0.903	2.4197	1	103.11	12.46	128.41
CO_2 + n-C_6H_{14}	0.0113	303.2	1.013	0.7561	0.9374	8.6703	0.9715	10.3093	1.0001	755.90	28.49	999.75
CO_2 + c-C_6H_{12}	0.00759	298.2	1.013	0.8732	1.8064	1.5005	0.9144	2.8019	1	48.12	4.72	55.11
CO_2 + C_6H_6	0.00912	298.2	1.013	0.8770	1.5099	2.7258	0.9543	4.4208	1	169.08	8.81	192.79
CO_2 + CH_3OH	0.00643	298.2	1.013	0.8349	2.0384	53.9653	0.9969	129.6644	1.0001	5227.28	19.41	6261.18
CO_2 + C_2H_5OH	0.00728	298.2	1.013	0.9230	1.9906	20.516	0.9962	43.51	1.0001	1925.27	7.93	2085.78
CO_2 + CS_2	0.003785	281.65	1.013	0.7601	4.6829	0.5181	0.531	1.6731	1	48.85	30.14	64.27
CO_2 + CS_2	0.003538	289.7	1.013	0.6642	3.5955	0.754	0.5488	2.2114	1	25.57	17.37	38.50
CO_2 + CS_2	0.00328	298.15	1.013	0.5317	2.5448	1.555	0.6949	5.1058	1	53.50	30.70	100.64

Table A11-3. Results of computer calculations using the AGAPE method, isothermal case.

Method	Experimental			Calculated from experimental data assuming $\gamma_2 = 1.0$		MHV2 isothermal				ERRORS MHV2 isothermal	% MHV2- "y"exp	% MHV2- "y"exp
										ΔP	Δy	$\Delta \gamma_1$
Mixture	x_1	T exp (K)	P exp (10^5 Pa)	y_1	γ_1	P cal MHV2 (10^5 Pa)	y_1	γ_1	γ_2			
$C_3H_8 + C_6H_6$	0.0813	283.15	1.013	0.9455	1.8696	1.2676	0.9528	2.5507	1.0125	25.1309	0.7716	32.2009
$C_3H_8 + C_6H_6$	0.0581	298.2	1.013	0.8831	1.6576	1.3618	0.9069	2.4556	1.0057	34.4332	2.6928	17.8455
$C_3H_8 + C_6H_6$	0.037	323.15	1.013	0.6603	1.0687	1.5786	0.7703	2.1818	1.0019	55.8385	16.6653	47.7173
$C_3H_8 + C_6H_6$	0.0255	343.15	1.013	0.3023	0.4703	15.1988	0.0265	1.9665	1.0007	1400.3702	91.2353	3131.662
C_3H_8 + n-C_6H_{14}	0.336	258.15	1.013	0.6295	0.6583	1.5280	0.9825	1.1183	1.038	50.8372	56.0830	132.0936
C_3H_8 + n-C_6H_{14}	0.188	278.15	1.013	0.9370	0.9254	1.1602	0.9404	1.1248	1.0082	14.5283	0.3674	25.3706
C_3H_8 + n-C_6H_{14}	0.138	288.2	1.013	0.8907	0.9031	1.1521	0.8967	1.1083	1.0034	13.7281	0.6779	27.5692
C_3H_8 + n-C_6H_{14}	0.116	298.2	1.013	0.8237	0.7637	1.2757	0.8503	1.0793	1.0017	25.9311	3.2326	67.0301
C_3H_8 + n-C_6H_{14}	0.0675	323.15	1.013	0.8661	2.8536	1.5260	0.6545	1.0025	1	50.6372	24.4350	46.5251
$C_3H_8 + CH_3OH$	0.02039	273.2	1.0084	0.9605	10.1288	1.3355	0.9695	15.5771	1.0021	32.4339	0.9360	86.8152
$C_3H_8 + CH_3OH$	0.004988	298.2	0.6186	0.7263	9.5646	0.6880	0.7535	12.3568	1.0001	11.2184	3.7394	92.8068
$C_3H_8 + CH_3OH$	0.00704	298.2	0.7974	0.7883	9.4791	0.8937	0.8095	12.153	1.0002	12.0751	2.6954	90.5720
$C_3H_8 + CH_3OH$	0.009569	298.2	1.0127	0.8337	9.3674	1.1399	0.8501	11.0977	1.0004	12.5611	1.9721	87.8311
$C_3H_8 + CH_3OH$	0.0115	298.2	1.013	0.8339	7.7997	1.2970	0.8797	10.6366	0.9973	28.0316	5.4889	83.3716
$C_3H_8 + CH_3OH$	0.003232	323.2	1.0111	0.4503	8.3185	0.9859	0.4354	8.7978	1	2.4931	3.3079	88.1482
$C_3H_8 + C_2H_5OH$	0.01497	273.2	0.413	0.9616	5.6562	0.4458	0.9641	7.5738	1.0006	7.9492	0.2585	92.1178
$C_3H_8 + C_2H_5OH$	0.02706	273.2	0.7093	0.9779	5.4649	0.7559	0.9788	7.0902	1.0021	6.5677	0.0881	86.1684
$C_3H_8 + C_2H_5OH$	0.04054	273.2	1.016	0.9848	5.2622	1.0670	0.9849	6.6041	1.0045	5.0150	0.0082	79.7244
$C_3H_8 + C_2H_5OH$	0.005089	298.2	0.331	0.7628	5.2753	0.3151	0.7474	5.6884	1.0001	4.7974	2.0233	94.0265
$C_3H_8 + C_2H_5OH$	0.01003	298.2	0.5699	0.8629	5.2126	0.5370	0.8514	5.5676	1.0002	5.7690	1.3305	89.6977
$C_3H_8 + C_2H_5OH$	0.01434	298.2	0.773	0.8994	5.1542	0.7245	0.8897	5.4654	1.0004	6.2777	1.0790	85.9441
$C_3H_8 + C_2H_5OH$	0.01941	298.2	1.007	0.9232	5.0919	0.9393	0.9147	5.3485	1.0008	6.7247	0.9234	81.5536
$C_3H_8 + C_2H_5OH$	0.0228	298.2	1.013	0.9237	4.3573	1.0791	0.9257	5.2722	1.0011	6.5263	0.2183	75.2346
$C_3H_8 + C_2H_5OH$	0.003201	323.15	0.5493	0.4643	4.7095	0.4965	0.402	4.2189	1	9.6136	13.4118	89.4576

Table A11-4. Results of computer calculations using the MHV2 method, isothermal case (continued over).

Method	Experimental			Calculated from experimental data assuming γ_2 = 1.0		MHV2 isothermal				ERRORS MHV2 isothermal	% MHV2- "y"exp	% MHV2- "y"exp
Mixture	x_1	T exp (K)	P exp (10^5 Pa)	y_1	γ_1	P cal MHV2 (10^5 Pa)	y_1	γ_1	γ_2	Δ P	Δ y	$\Delta \gamma_1$
$C_3H_8 + C_2H_5OH$	0.006342	323.15	0.7951	0.6309	4.6762	0.6910	0.5689	4.1741	1	13.0881	9.8301	85.2222
$C_3H_8 + C_2H_5OH$	0.009245	323.15	1.0191	0.7129	4.6455	0.8694	0.6545	4.149	1.0001	14.6925	8.1885	81.2859
$n\text{-}C_4H_{10} + n\text{-}C_6H_{14}$	0.737	278.15	1.013	0.9796	1.0805	0.9413	0.9743	1.0079	1.0901	7.0771	0.5416	12.8849
$n\text{-}C_4H_{10} + n\text{-}C_6H_{14}$	0.441	288.2	1.013	0.9291	1.2061	0.8684	0.9095	1.0366	1.031	14.2788	2.1061	28.0023
$n\text{-}C_4H_{10} + n\text{-}C_6H_{14}$	0.386	298.2	1.013	0.8776	0.9426	1.0801	0.8755	1.0366	1.0193	6.6263	0.2348	14.5856
$n\text{-}C_4H_{10} + n\text{-}C_6H_{14}$	0.199	323.15	1.013	0.5729	0.5867	1.4003	0.6765	1.0282	1.0022	38.2341	18.0737	138.6868
$n\text{-}C_4H_{10} + CH_3OH$	0.01651	298.2	0.6594	0.7462	12.1981	0.9626	0.8242	20.4635	1.0021	45.9793	10.4478	92.1087
$n\text{-}C_4H_{10} + CH_3OH$	0.0241	298.2	0.8474	0.8041	11.5703	1.2200	0.8611	18.3723	1.0043	43.9642	7.0900	89.4562
$n\text{-}C_4H_{10} + CH_3OH$	0.0398	298.2	1.013	0.8387	8.7369	1.6009	0.8942	14.9305	1.0111	58.0390	6.6162	81.6761
$n\text{-}C_4H_{10} + CH_3OH$	0.03171	298.2	1.0159	0.8378	10.9869	1.4267	0.8811	16.5734	1.0073	40.4327	5.1632	87.0150
$n\text{-}C_4H_{10} + CH_3OH$	0.0192	308.2	1.0007	0.7249	11.4582	1.4165	0.8004	18.21	1.0028	41.5533	10.4132	87.6375
$n\text{-}C_4H_{10} + CH_3OH$	0.008075	323.2	1.009	0.4518	11.3405	1.3132	0.5752	19.4958	1.0005	30.1459	27.3207	88.4205
$n\text{-}C_4H_{10} + C_2H_5OH$	0.01517	298.2	0.3173	0.7551	6.4731	0.3567	0.7785	8.1441	1.0009	12.4059	3.1002	94.4900
$n\text{-}C_4H_{10} + C_2H_5OH$	0.02334	298.2	0.4344	0.8227	6.2771	0.4833	0.837	7.6568	1.0021	11.2616	1.7436	92.3002
$n\text{-}C_4H_{10} + C_2H_5OH$	0.02999	298.2	0.5244	0.8540	6.1209	0.5755	0.8635	7.2928	1.0034	9.7494	1.1082	90.5974
$n\text{-}C_4H_{10} + C_2H_5OH$	0.0344	298.2	0.5824	0.8692	6.0329	0.6323	0.876	7.066	1.0045	8.5625	0.7798	89.5197
$n\text{-}C_4H_{10} + C_2H_5OH$	0.05144	298.2	0.7865	0.9048	5.6711	0.8228	0.9052	6.2862	1.0098	4.6102	0.0393	85.4920
$n\text{-}C_4H_{10} + C_2H_5OH$	0.07092	298.2	0.9859	0.9257	5.2747	0.9930	0.922	5.5505	1.018	0.7186	0.3972	81.1747

Table A11-4. Results of computer calculations using the MHV2 method, isothermal case (continued over).

Method	Experimental			Calculated from experimental data assuming γ_2 = 1.0		MHV2 isothermal				ERRORS MHV2 isothermal	% MHV2- "y"exp	% MHV2- "y"exp
Mixture	x_1	T exp (K)	P exp (10^5 Pa)	y_1	γ_1	P cal MHV2 (10^5 Pa)	y_1	γ_1	γ_2	Δ P	Δ y	$\Delta \gamma_1$
n-C_4H_{10} + C_2H_5OH	0.0815	298.2	1.013	0.9282	4.7222	1.0690	0.9278	5.2075	1.0238	5.5260	0.0472	77.3626
n-C_4H_{10} + C_2H_5OH	0.008298	308.2	0.3106	0.5592	6.3486	0.3384	0.5908	7.8798	1.0003	8.9586	5.6456	94.6693
n-C_4H_{10} + C_2H_5OH	0.01484	308.2	0.4401	0.6917	6.2307	0.4803	0.712	7.4918	1.0009	9.1299	2.9283	92.2917
n-C_4H_{10} + C_2H_5OH	0.02198	308.2	0.574	0.7654	6.0705	0.6201	0.7775	7.1013	1.0019	8.0329	1.5817	89.7849
n-C_4H_{10} + C_2H_5OH	0.04476	308.2	0.959	0.8628	5.6151	0.9849	0.8609	6.0484	1.0074	2.6985	0.2231	82.4601
n-C_4H_{10} + C_2H_5OH	0.00521	323.1	0.4504	0.3479	6.0501	0.4701	0.3704	7.2379	1.0001	4.3845	6.4807	92.2290
n-C_4H_{10} + C_2H_5OH	0.01218	323.1	0.6499	0.5513	5.9162	0.6829	0.5675	6.8501	1.0006	5.0824	2.9458	88.4565
n-C_4H_{10} + C_2H_5OH	0.01716	323.1	0.7874	0.6314	5.8287	0.8238	0.6413	6.5966	1.0011	4.6193	1.5612	85.8670
n-C_4H_{10} + C_2H_5OH	0.02442	323.1	0.9779	0.7055	5.6825	1.0112	0.708	6.2529	1.0023	3.4077	0.3557	82.2045
CO_2 + n-C_6H_{14}	0.0126	293.2	1.013	0.8423	1.1786	1.1460	0.8545	1.6648	1.0001	13.1279	1.4491	2.7636
CO_2 + n-C_6H_{14}	0.0119	298.2	1.013	0.8030	1.0594	1.1855	0.8239	1.5831	1.0001	17.0289	2.6048	11.9057
CO_2 + n-C_6H_{14}	0.0113	303.2	1.013	0.7561	0.9374	1.2331	0.7908	1.5091	1	21.7300	4.5905	31.5439
CO_2 + C_6H_6	0.00912	298.2	1.013	0.8770	1.5099	1.3415	0.9027	2.603	1.0001	32.4327	2.9270	11.1497
CO_2 + CH_3OH	0.00643	298.2	1.013	0.8349	2.0384	1.2493	0.8634	3.3423	1	23.3304	3.4172	38.7091
CO_2 + C_2H_5OH	0.00728	298.2	1.013	0.9230	1.9906	0.9869	0.9187	2.5546	1	2.5760	0.4710	50.4216

Table A11-4. Results of computer calculations using the MHV2 method, isothermal case.

Method	Experimental			Calculated from exp. data ass. γ_2 = 1.0		Reference solvent					ERRORS Ref. Sol.	% Ref. Sol.- "y"exp	% Ref. Sol. "y" exp	% Ref. Sol.- "y"exp
Mixture	x_1	T exp (K)	P exp (10^5 Pa)	y_1	γ_1	P (10^5 Pa)	x_1	y_1	γ_1	γ_2	Δ P	Δ y	$\Delta \gamma_1$	Δx_1
CO_2 + n-C_6H_{14}	0.0126	293.2	1.013	0.8423	1.1786	1.0002	0.0125	0.8423	1.1891	1.0001	1.2636	0.0007	0.8946	0.7937
CO_2 + n-C_6H_{14}	0.0119	298.2	1.013	0.8030	1.0594	1.0846	0.01172	0.8204	1.1929	1.0001	1.2636	0.0007	0.8946	0.7937
CO_2 + n-C_6H_{14}	0.0113	303.2	1.013	0.7561	0.9374	1.1938	0.01113	0.7958	1.1963	1.0001	7.0681	2.1689	12.6040	1.5126
CO_2 + c-C_6H_{12}	0.00759	298.2	1.013	0.8732	1.8064	1.2525	0.00762	0.7211	1.8626	1.0001	17.8480	5.2517	27.6156	1.5044
CO_2 + C_6H_6	0.00912	298.2	1.013	0.8770	1.5099	1.0252	0.00977	0.879	1.4497	1.0001	23.6426	17.4192	3.1130	0.3953
CO_2 + CH_3OH	0.00643	298.2	1.013	0.8349	2.0384	1.4147	0.00547	0.6227	2.5301	1.0001	1.2043	0.2247	3.9865	7.1272
CO_2 + C_2H_5OH	0.00728	298.2	1.013	0.9230	1.9906	0.9663	0.00625	0.9197	2.2334	1.0001	39.6545	25.4136	24.1236	14.9300

Table A11-5. Results of computer calculations using the reference method.

A11.2 Prediction of solubilities using the solubility parameters

solute	298.15 K	T_C (K)	T_r	P_C (10^5 Pa)	f^L_2/P_C (curve)	v^L (cm^3/mol)
compound	solubility parameter $(J/cm^3)^{0.5}$				polynomium	
methane	11.6	190.4	1.565913866	46	3.767124717	52
argon	10.9	150.8	1.977122016	48.7	5.533259274	57.1
nitrogen	5.3	126.2	2.36251981	33.9	8.289209492	32.4
oxygen	8.18	154.6	1.928525226	50.4	5.390052184	33
carbon dioxide	12.3	304.1	0.980434068	73.8	0.588418426	55
carbon monoxide	6.4	132.9	2.243416102	35	6.798024082	32.1
ethylene	13.5	282.4	1.055771955	50.4	0.831323148	65
ethane	13.5	305.4	0.976260642	48.8	0.576781246	70
n-propane	13.1	369.8	0.80624662	$42.5^{1)}$	0.204661693	92.21
n-butane	13.7	425.2	0.701199436	$38^{1)}$	$0.08^{2)}$	101.15

Table A11-6. Parameters to be used in the regular solutions theory (equation (3.18)).

The values of the solubility parameters are from Table 4-22, the critical pressures and the critical temperatures are from Reid et al. (1987), while the molar volumes are from Prausnitz et al. (1986). The molar volumes for propane and n-butane (marked 1) are calculated from the Yen-Woods method (1966). The value of the fugacity of the hypothetical liquid is from a curve-fitting expression obtained by reading points from the curve in Prausnitz and Shair (1961) and redrawing the curve. The fugacity of the hypothetical liquid for n-butane (marked 2) is read from the curve in Yen and McKetta (1962).

In Figure A11.4 the points ■ represent the values read from the curve in Prausnitz and Shair and the continuous line (—) is the best linear fitted line between the points

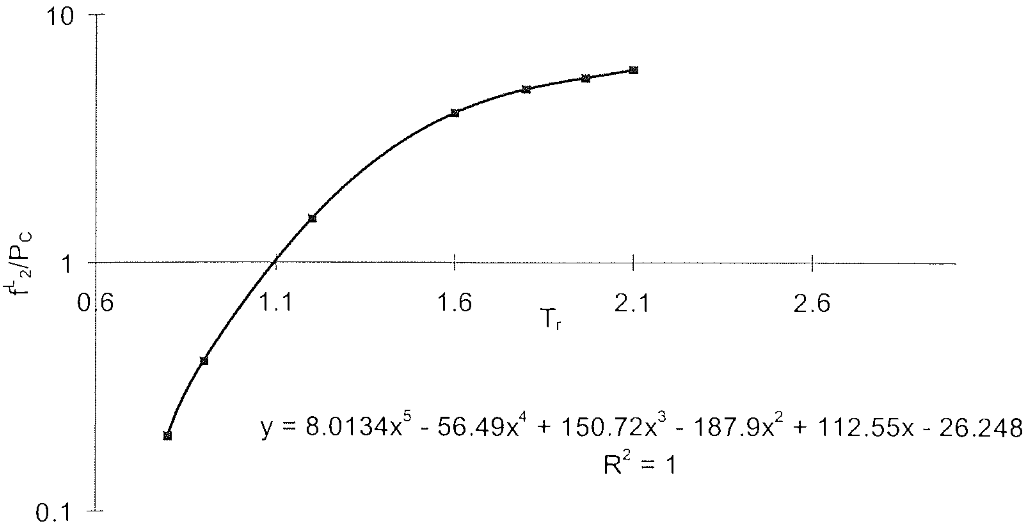

Figure A11.4. The fugacity divided by the critical pressure of the hypothetical liquid (solutes) as a function of the reduced temperature (reproduced from Prausnitz and Shair, 1961).

Appendix 12 - Results of fitting the like London potential

A12.1 Results of the vapour pressure calculations

The equation for the saturated vapour pressure as a function of temperature (from Reid et al., 1987)

$$\ln\left(\frac{P^S}{P_C}\right) = \left(\frac{1}{1 - \frac{T}{T_C}}\right)\left[A\left(1 - \frac{T}{T_C}\right) + B\left(1 - \frac{T}{T_C}\right)^{1.5}\right] + \left(\frac{1}{1 - \frac{T}{T_C}}\right)\left[C\left(1 - \frac{T}{T_C}\right)^{3} + D\left(1 - \frac{T}{T_C}\right)^{6}\right] \qquad (A12.1)$$

This equation is the so-called Wagner equation, and to calculate the saturated vapour pressure beyond the critical temperature, Reid et al. (1987) recommend that this equation is extrapolated, but only in the temperature interval from the $0.5 < T/T_C < 1.0$. Extrapolation beyond $0.5 < T/T_C$ is not recommended at all.

The Wagner equations for respectively methane and ethane have used to calculate the saturated vapour pressures (P^S in Tables A12-1 and A12-2) and then extrapolated within the recommended temperature interval. The results are shown below.

CH_4	A	-6.00435	
methane	B	1.18885	
	C	-0.83408	
	D	-1.22833	
	T_C	190.4	K
	P_C	46	bar
T (K)	$1/T_r=T_c/T$	P^S (10^5 Pa)	ln (P^S/P_c)
120	1.58666667	1.93153441	-3.1703267
130	1.46461538	3.70321269	-2.5194407
140	1.36	6.46018586	-1.9629833
150	1.26933333	10.4720251	-1.479934
160	1.19	16.0227307	-1.054633
170	1.12	23.4217582	-0.674976
180	1.05777778	33.0371647	-0.3310083
190	1.00210526	45.4273965	-0.012526
190.4	1	46	0

Table A12-1. Results of calculations of the saturated vapour pressure for **methane**. Coefficients from Reid et al. (1987)

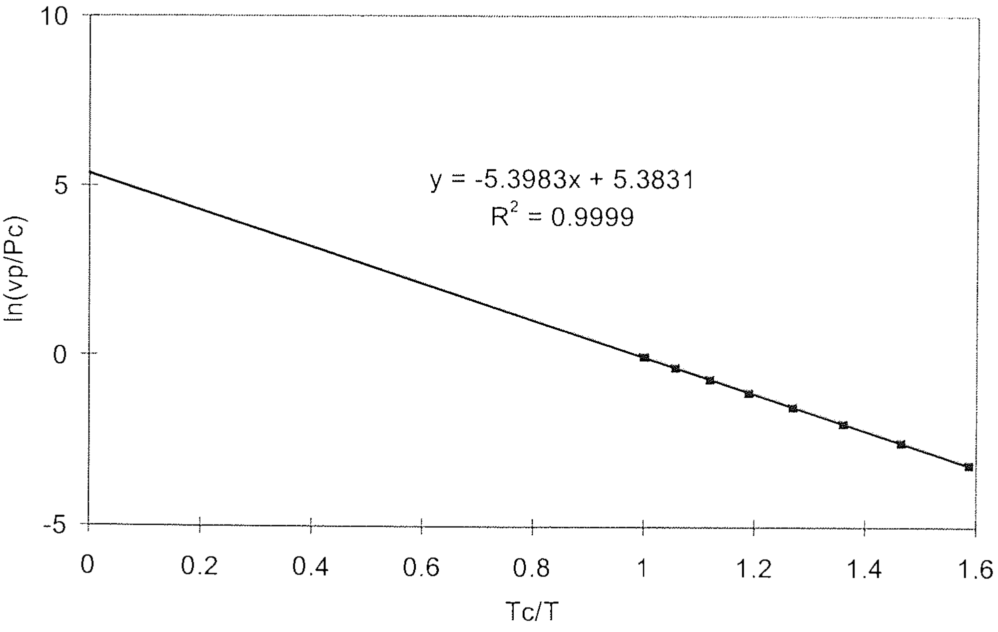

Figure A12.1. The logarithm of the reduced vapour pressure of **methane** as a function of reciprocal reduced temperature.

The best linear fit gives the equation

$$\ln\left(\frac{P^S}{P_C}\right) = -5.3983\left(\frac{T_C}{T}\right) + 5.3831 \qquad \text{(A12.2)}$$

where P^S is in 10^5Pa and T is in K.

Using this equation, the saturated vapour pressure of methane at 298.15 K is obtained to be 318.742 10^5 Pa.

C_2H_6	A	-6.34307	
ethane	B	-1.0163	
	C	-1.19116	
	D	-2.03539	
	T_C	305.4	K
	P_C	48.2	bar
T (K)	$1/T_r=T_c/T$	P^S (10^5 Pa)	ln (P^S/P_c)
170	1.796470588	0.431875334	-4.72735
180	1.696666667	0.791326384	-4.12178
190	1.607368421	1.352246427	-3.58596
200	1.527	2.180500234	-3.10818
210	1.454285714	3.348971296	-2.67908
220	1.388181818	4.936105319	-2.29115
230	1.327826087	7.024734076	-1.93829
240	1.2725	9.701358377	-1.61546
250	1.2216	13.05605498	-1.31848
260	1.174615385	17.18320993	-1.0438
270	1.131111111	22.18342124	-0.78839
280	1.090714286	28.16732803	-0.54957
290	1.053103448	35.26354288	-0.32488
300	1.018	43.64029285	-0.11175
305.4	1	48.8	0
305	47.79839212	0.00327869	1.67941329

Table A12-2. Results of calculations of the saturated vapour pressure for **ethane**. Coefficients from Reid et al. (1987)

The best linear fit gives the equation

$$\ln\left(\frac{P^S}{P_C}\right) = -5.9010\left(\frac{T_C}{T}\right) + 5.8935 \qquad \text{(A12.3)}$$

where P^S is in 10^5Pa and T is in K.

Using this equation, the saturated vapour pressure of ethane at 307.94 K is obtained to be 51.891 10^5 Pa.

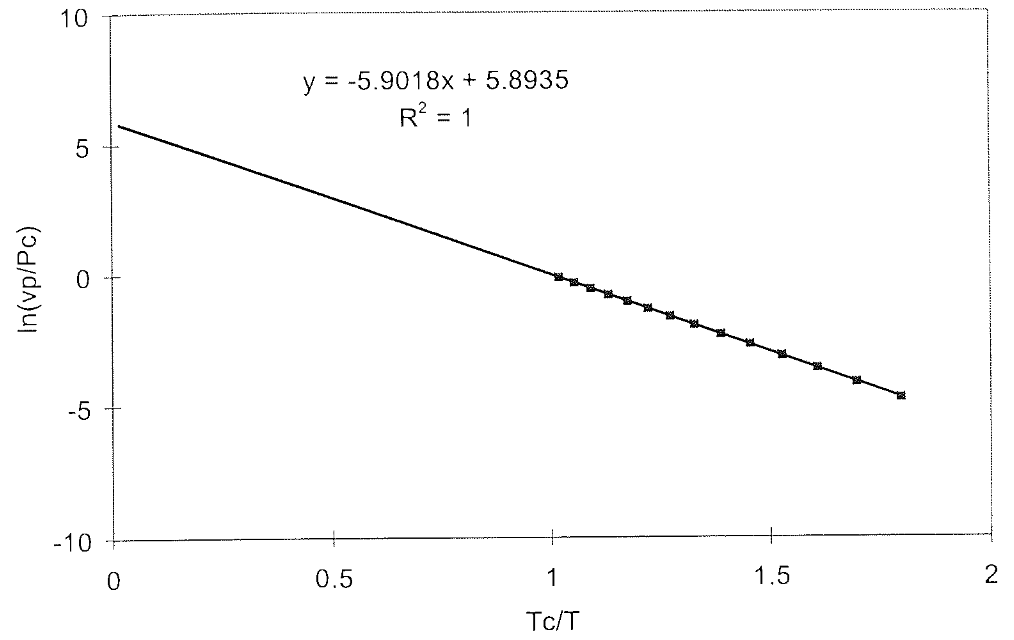

Figure A12.2. The logarithm of the reduced saturated vapour pressure of **ethane** as a function of reciprocal reduced temperature.

A12.2 Fitting of the like potential

The results of the calculations are shown in Tables A12-3 to A12-12. The first two columns display the like pair potential for component 1 and 2, respectively, then follows the unlike geometric mean pair potential. In column 4 are the values of the calculated unlike London pair potential, then follows the ratio of the unlike London pair potential to the unlike geometric mean pair potential (ratio = P12-GLP / P12-GM). The size parameter, r (ratio of the van der Waals volumes of the two components) is displayed in the sixth column. The last two columns contain the vapour mole fractions of component 1 and component 2, respectively.

All experimental data are from the relevant volume of IUPAC Solubility Data Series (Clever, 1979 (vol. 1), Clever, 1980 (vol. 4), Young, 1981 (vol. 5/6), Battino, 1981 (vol. 7), Hayduk, 1982 (vol. 9), Battino, 1982 (vol. 10), Hayduk, 1986 (vol. 24), and Clever and Young, 1987 (vol. 27/28)).

Mixture: benzene (1) - methane (2) at 298.15 K, 101.325 kPa pressure of methane and $x_2 = 0.00209$

iteration number	**P11 (E19 J)**	**P22 (E19 J)**	**P12-GM (E19 J)**	**P12-GLP (E19 J)**	**P12 ratio**	**r (ratio of van der Waals volumes)**	y_1	y_2
1	-0.093996	-0.00807	-0.0275	-0.0233	0.8473	0.354	0.8047	0.1099
2	-0.093996	-0.006	-0.02375	-0.01955	0.8231	0.354	0.9036	0.1099

Result after iteration number 2: $\gamma_2 = 1.5368$.

Table A12-3. Results of computer calculations using the PP program to fit the like potential for CH_4 in C_6H_6 - CH_4.

Mixture: *cyclo* hexane (1) - methane (2) at 298.15 K, 101.325 kPa pressure of methane and $x_2 = 0.00327$

iteration number	**P11 (E19 J)**	**P22 (E19 J)**	**P12-GM (E19 J)**	**P12-GLP (E19 J)**	**P12 ratio**	**r (ratio of van der Waals volumes)**	y_1	y_2
1	-0.091765	-0.00807	-0.0272	-0.0230	0.8457	0.2918	0.9498	0.1126
2	-0.091765	-0.006	-0.02346	-0.01926	0.8210	0.2918	1.0467	0.1126
3	-0.091765	-0.0175	-0.0400	-0.03587	0.8952	0.2918	0.8169	0.1126
4	-0.091765	-0.011	-0.03177	-0.02757	0.8678	0.2918	0.8730	0.1126
5	-0.091765	-0.01	-0.03029	-0.02609	0.8614	0.2918	0.8936	0.1126

Result after iteration number 5: $\gamma_2 = 0.9792$.

Table A12-4. Results of computer calculations using the PP program to fit the like potential for CH_4 in c-C_6H_{12}- CH_4.

Mixture: methane (1) - n-hexane (2) at 298.15 K, 101.325 kPa pressure of methane and $x_1 = 0.00508$.

iteration number	**P11 (E19 J)**	**P22 (E19 J)**	**P12-GM (E19 J)**	**P12-GLP (E19 J)**	**P12 ratio**	**r (ratio of van der Waals volumes)**	y_1	y_2
1	-0.00807	-0.087819	-0.0266	-0.0224	0.8422	3.9871	1.0125	0.1651
2	-0.006	-0.087819	-0.02375	-0.01875	0.8170	3.9871	1.1019	0.1651
3	-0.01	-0.087819	-0.02963	-0.02543	0.8583	3.9871	0.9619	0.1651
4	-0.04	-0.087819	-0.05927	-0.05507	0.92914	3.9871	1.1797	0.1651
5	-0.02	-0.087819	-0.04191	-0.03771	0.8998	3.9871	0.9125	0.1651
6	-0.015	-0.087819	-0.03629	-0.03209	0.8843	3.9871	0.9079	0.1651
7	-0.0175	-0.087819	-0.03920	-0.03500	0.8929	3.9871	0.9050	0.1651
8	-0.0125	-0.087819	-0.03313	-0.02893	0.8732	3.9871	0.9249	0.1651
9	-0.025	-0.087819	-0.046856	-0.042656	0.9104	3.9871	0.9499	0.1651

Table A12-5. Results of computer calculations using the PP program to fit the like potential for CH_4 in CH_4 - n-C_6H_{14}.

Mixture: methane (1) - n-butane (2) at 298.15 K, 2.76 kPa total pressure and $x_1 = 0.0036$

iteration number	P11 (E19 J)	P22 (E19 J)	P12-GM (E19 J)	P12-GLP (E19 J)	P12 ratio	r (ratio of van der Waals volumes)	y_1	y_2
1	-0.00807	-0.056466	-0.02135	-0.01715	0.8032	2.7921	0.4815	0.2103
2	-0.010	-0.056466	-0.02376	-0.1956	0.82325	2.7921	0.4517	0.2103
3	-0.020	-0.056466	-0.0336	-0.0294	0.875	2.7921	0,4129	0.2103
4	-0.04	-0.056466	-0.04753	-0.04333	0.9116	2.7921	0.5421	0.2103

Table A12-6. Results of computer calculations using the PP program to fit the like potential for CH_4 in CH_4 - n-C_4H_{10}.

Mixture: methane (1) - carbon disulphide (2) at 298.15 K, 101.325 kPa pressure of methane and $x_1 = 0.01312$.

iteration number	P11 (E19 J)	P22 (E19 J)	P12-GM (E19 J)	P12-GLP (E19 J)	P12 ratio	r (ratio of van der Waals volumes)	y_1	y_2
1	-0.00807	-0.075917	-0.022475	-0.02375	0.9596	1.8224	4.9278	0.3150
2	-0.04	-0.075917	-0.05511	-0.05411	0.9819	1.8224	2.6924	0.3150
3	-0.01	-0.075917	-0.02755	-0.02655	0.9637	1.8224	4.3387	0.3150
4	-0.02	-0.075917	-0.03897	-0.03797	0.9743	1.8224	3.0514	0.3150
5	-0.08	-0.075917	-0.07793	-0.07693	0.9872	1.8224	3.2442	0.3150

Table A12-7. Results of computer calculations using the PP program to fit the like potential for CH_4 in CH_4 - CS_2.

Mixture: carbon tetrachloride(1) - methane (2) at 298.14 K and 101.325 kPa pressure of methane and $x_2 = 0.002818$.

iteration number	P11 (E19 J)	P22 (E19 J)	P12-GM (E19 J)	P12-GLP (E19 J)	P12 ratio	r (ratio of van der Waals volumes)	y_1	y_2
1	-0.092617	-0.00807	-0.02734	-0.02554	0.9342	2.9045	498.7	0.1289
2	-0.092617	-0.02	-0.04304	-0.04124	0.9582	2.9045	21.6	0.1289
3	-0.092617	-0.04	0.06087	-0.05907	0.9704	2.9045	1.8926	0.1289
4	-0.092617	-0.06	-0.07455	-0.07275	0.9759	2.9045	0.6859	0.1289
5	-0.092617	-0.055	-0.07137	-0.06957	0.9748	2.9045	0.8114	0.1289
6	-0.092617	-0.057	-0.07266	-0.07086	0.9752	2.9045	0.7551	0.1289
7	-0.092617	-0.053	-0.07006	-0.06826	0.9743	2.9045	0.8805	0.1289

Result after iteration number 7: $\gamma_2 = 1.1407$.

Table A12-8. Results of computer calculations using the PP program to fit the like potential for CH_4 in CCl_4 - CH_4.

Mixture: *cyclo* hexane (1) - n-propane (2) at 298.15 K, 101.1325 kPa pressure of n-propane and $x_2 = 0.0896$.

iteration number	P11 (E19 J)	P22 (E19 J)	P12-GM (E19 J)	P12-GLP (E19 J)	P12 ratio	r (ratio of van der Waals volumes)	y_1	y_2
1	-0.091765	-0.036630	-0.057977	-0.057121	0.9852	0.6403	0.8019	0.1029
2	-0.091765	-0.03	-0.05247	-0.051613	0.9837	0.6403	0.8411	0.1029
3	-0.091765	-0.025	-0.047897	-0.047041	0.9821	0.6403	0.8998	0.1209

Result after iteration number 3: $\gamma_2 = 1.2196$

Table A12-9. Results of computer calculations using the PP program to fit the like potential for C_3H_8 in c-C_6H_{12} - C_3H_8.

Mixture: benzene (1) - n-propane (2) at 310.93 K, 101.1325 kPa pressure of methane and $x_2 = 0.0397$.

iteration number	P11 (E19 J)	P22 (E19 J)	P12-GM (E19 J)	P12-GLP (E19 J)	P12 ratio	r (ratio of van der Waals volumes)	y_1	y_2
1	-0.091729	-0.033103	-0.055104	-0.053062	0.9629	0.7769	0.6279	0.1641
2	-0.091729	-0.030	-0.052458	-0.0504163	0.9611	0.7769	0.6556	0.1641
3	-0.091729	-0.028	-0.050680	-0.04864	0.9597	0.7769	0.6790	0.1641
4	-0.091729	-0.025	-0.047888	-0.045846	0.9574	0.7769	0.7235	0.1641
5	-0.091729	-0.020	-0.042832	-0.04079	0.9523	0.7769	0.8372	0.1641

Result after iteration number 5: $\gamma_2 = 2.1109$.

Table A12-10. Results of computer calculations using the PP program to fit the like potential for C_3H_8 in C_6H_6 - C_3H_8.

Mixture: *cyclo* hexane (1) - ethane (2) at 307.95 K, 101.1325 kPa pressure of ethane and $x_2 = 0.02055$.

iteration number	P11 (E19 J)	P22 (E19 J)	P12-GM (E19 J)	P12-GLP (E19 J)	P12 ratio	r (ratio of van der Waals volumes)	y_1	y_2
1	-0.090099	-0.02881	-0.045334	-0.043031	0.9492	0.46592	0.9795	0.1597
2	-0.090099	-0.025	-0.04746	-0.045157	0.95148	0.46592	0.9634	0.1597
3	-0.090099	-0.030	-0.05199	-0.049687	0.9557	0.46592	0.9478	0.1597
4	-0.090099	-0.040	-0.060033	-0.05773	0.96164	0.46592	0.9713	0.1597

Table A12-11. Results of computer calculations using the PP program to fit the like potential for C_2H_6 in c-C_6H_{12} - C_2H_6.

Mixture: methane (1) - n-propane (2) at 213.71 K, 144.9 kPa pressure of methane and $x_1 = 0.0205$.

iteration number	**P11 (E19 J)**	**P22 (E19 J)**	**P12-GM (E19 J)**	**P12-GLP (E19 J)**	**P12 ratio**	**r (ratio of van der Waals volumes)**	y_1	y_2
1	-0.0807	-0.053922	-0.06597	-0.06397	0.9697	2.1945	1.6347	0.2331
2	-0.04	-0.053922	-0.04644	-0.0444	0.9569	2.1945	1.1927	0.2331
3	-0.01	-0.053922	-0.02322	-0.02122	0.9139	2.1945	1.1145	0.2331
4	-0.001	-0.053922	-0.00734	-0.00534	0.7276	2.1945	3.1586	0.2331
5	-0.005	-0.053922	-0.01642	-0.01442	0.8782	2.1945	1.5193	0.2331
6	-0.02	-0.053922	-0.03284	-0.03084	0.9391	2.1945	0.9675	0.2331

Table A12-12. Results of computer calculations using the PP program to fit the like potential for CH_4 in CH_4 - n- C_6H_{14}.

Appendix 13 - Results of heat of vaporization calculations

A13.1 Introduction

The theoretical basis for the AGAPE theory has been described in chapter 2. The calculations use either the heat of vaporization or the molar volume to calculate the equilibrium separation for the pure compounds at the actual temperature. The equilibrium separation is a crucial parameter in the AGAPE calculations, mainly because it occurs raised to the power of -6, thus an inaccurate equilibrium separation creates even greater errors in the final results.

It is therefore important to investigate how correct the chosen methods for obtaining the heat of vaporization and the molar volume are. That for heat of vaporization is examined first, then that for the molar volume. Both are extended beyond the original areas of applicability.

This investigation concentrates on a fundamental parameter in the GLP theory and is therefore not directly related to solubility. Thus do Appendices 13 and 14 contain this investigation.

A13.2 Heat of vaporization

A13.2.1 Polar compounds and compounds containing hydrogen bonding

The GLP theory enables us to calculate vapour-liquid equilibria and excess Gibbs free energy (G^E) for binary and multicomponent mixtures from a generalized London potential with some limitations. As we have already seen they are small compounds (less than C_6), non-polar compounds, no hydrogen bonding, low pressure, and temperature and pressure below the critical temperature and pressure of the pure compounds.

If the theory is to be extended, we need to be able to calculate the heat of vaporization for polar compounds and compounds containing hydrogen bonding. This problem has been investigated by carrying out *ab initio* calculations for the four components i.e. methanol, ethanol, acetone, and acetic acid.

These components are both polar and contain hydrogen bondings. They were chosen as the smallest alcohols and organic acids. The work on polar compounds/compounds containing hydrogen bondings began for small molecules, because the equilibrium separation had to be calculated by hand, and the calculations were easiest for small molecules.

The intention was to carry out predictions for these four components as if they were non-polar. This means that prediction of VLE data from AGAPE was carried out without taking into account that the components are in fact polar and with hydrogen bonding. From these calculations it was hoped to be able to account for the calculation for the polar effect and the hydrogen bonding effect.

A program calculating the latent heat of vaporization at a given temperature for the specific compound in the AGAPE database, GEX.DAT was written and was included as a separate option in the existing menu of AGAPE programs.

The program was written to calculate the latent heat of vaporization by three different methods, as follows.

A13.2.2 The POT method

The first is the POT method, where the name indicates the connection with the gereralized London potential. The program calculates the equilibrium separation from molar volume, using the equation (2.80) (given in section 2.11). From that the like pair potentials for the pure component (equation (2.79)) is calculated, and then the latent heat of vaporization (equation (2.81)). In fact the program follows the same method as described by Homer and Mohammadi (1987b).

The molecular volume is related to the molar volume by L, Avogadro's number. The molar volume can be calculated as a function of temperature by a method from Yen and Woods (1966) using equations (4.11) and (4.12).

It is worth noticing that this approach is different from the calculation of the equilibrium separation, R^A, as described in section 2.11, where the problem, in order to determine the activity coefficients, was to determine the unlike pair of (London) potential from the equilibrium separation. This was solved calculating the equilibrium separation from the molar volume (using the Yen-Woods method) or from the heat of vaporization (using the Watson's correlation) at the given temperature.

The POT method calculates the heat of vaporization using the opposite approach. From a given temperature, the molar volume for the compound is calculated, and from that the equilibrium separation. This distance is used in equation (4.8).

This problem has been investigated by Mohammadi (1986, and Homer and Mohammadi, 1987b) in a similar manner. Their results were obtained from using the available experimental equilibrium separation (for the majority of the compounds at their freezing points) to calculate the heat of vaporization by inserting these intermolecular distances directly in equation (4.9). Their results obtained for the heat of vaporization were then compared with the experimental values at the melting points of the pure compounds. Despite the inconsistency in using values at the freezing points and the melting points, respectively, they obtained reasonably accurate results.

A13.2.3 Watson's correlation

The second method is Watson's correlation (Reid et al., 1987). The heat of vaporization ($\Delta Hvap_{,1}$) at the boiling point (T_1) is included in the AGAPE database. The program calculates the latent heat of vaporization ($\Delta Hvap_{,2}$) at another temperature (T_2) using Watson's correlation as described by equations (4.6) and (4.7).

A13.2.4 The Method of Daubert and Danner (1984)

The third method is the method by Daubert and Danner (1984). Daubert and Danner (1984) give for many compounds the coefficients A, B, C, D, and E in an equation for the heat of vaporization as a function of temperature.

In the method of Daubert and Danner (1984) the heat of vaporization is given by

$$\Delta H_{vap} = A^D(1 - T_r)^{e^D} \qquad (A13.1)$$

where e^D is defined as

$$e^D = B^D + C^D T_r + D^D T_r^2 + E^D T_r^3 \qquad (A13.2)$$

and the reduced temperature (T_r) as

$$T_r = T / T_c \qquad (A13.3)$$

A13.2.5 Results of the heat of vaporization calculations

The existing programs (VLE programs) have been modified to calculate the heat of vaporization for pure compounds. In the program the heat of vaporization is calculated from parameters used in VLE calculations (the POT method), by the Watson's correlation, and using the coefficients given by Daubert and Danner (1984). By using three alternative methods it could be possible to find terms for other parameters, and try to figure out their importance in connection to AGAPE. The parameter of particularly interest is R^A, and indirectly Φ_{ij}.

The heat of vaporization has been calculated for each of the following compounds:

- oxygen
- nitrogen
- benzene
- carbon tetrachloride
- methanol
- ethanol
- acetone
- acetic acid

at temperatures between the melting point and the critical temperature.

The last 4 compounds are chosen, because they are both polar and contain hydrogen bondings. The first four compounds are chosen among the compounds in Table 2-6, there are many experimental data on these compounds in the literature. The heat of vaporization for each compound is plotted together with experimental values (Perry and Green, 1984 and Reid et al, 1987) as a function of temperature in Figures A13-1 to A13-8.

For all the compounds the number of nearest neighbours z is set to 11.0. This value gave poor results for the polar compounds/compounds containing hydrogen bonding as shown on Figures A13-4 to A13-8. For these four compounds (methanol, ethanol, acetone, and acetic acid), the heat of vaporization has been calculated for z = 7.0, and z = 4.0 as well. These values of z are chosen after Moelwyn-Hughes (1971). He calculated the number of nearest neighbours for the liquid state from the potential energy. He found z = 7.0 for Hg, and z = 4.0 for water, that is a compound with hydrogen bondings. Homer and Mohammadi (1987b) used the value of z = 7.0 for Cl_2, SiF_4, SF_6, PCl_3, PBr_3, $AsCl_3$, and Hg. Therefore, the calculations have been carried out for z values of 7.0, and 4.0 for methanol, ethanol, acetone, and acetic acid.

compound	A	B	C	D
methanol	52.7	0.3776	-	-
ethanol	44.15	-0.4134	0.75362	-
acetone	49.17	1.036	-1.294	0.672
acetic acid	12.6	-1.11	0.063	1.142
benzene	50.73	0.7616	-0.5052	0.1564
carbon tetrachloride	38.784	-0.0736	-0.7385	-0.3192
nitrogen	9.43	1.201	-1.4822	0.7085
oxygen	8.04	-0.098	0.599	-0.189

Table A13-1. The coefficients A, B, C, and D to be used in equations (A13.1) and (A13.2) to calculate the heat of vaporization. From Daubert and Danner (1994).

T (K)	Hvap (kJ/mol), method by Daubert and Danner (1984)	Hvap (kJ/mol) Watson's correlation	Hvap (kJ/mol) POT method	Hvap (kJ/mol) exp. data (Perry and Green, 1984)
192	36.5	37.21	32.05	
194	36.44	37.13	31.96	
196	36.39	37.06	31.87	
198	36.33	36.98	31.78	
200	36.27	36.9	31.69	
210	35.96	36.5	31.25	
220	35.63	36.1	30.8	
230	35.29	35.69	30.36	
240	34.93	35.27	29.91	
253.15				34.72
260	34.16	34.4	29	
273.1				33.51
280	33.32	33.5	28.08	
300	32.41	32.56	19.43	
313.15				30.87
350	29.83	29.98	17.19	29.88
353.15				27.65
393.15				27.01
400	26.76	26.98	16.29	
433.15				24.43
450	23.04	23.31	14.5	
473.1				21.09
500	18.13	18.31	12.37	
513.15				17.36
550	8.33	8.01	6.91	

Table A13-2. Heat of vaporization for **carbon tetrachloride** by three different methods as a function of temperature

T (K)	Hvap (kJ/mol), method by Daubert and Danner (1984)	Hvap (kJ/mol) Watson's corr	Hvap (kJ/mol) GLP , z=11	Hvap (kJ/mol) GLP , z=4	Hvap (kJ/mol) GLP , z=7	Hvap (kJ/mol) exp. data (Perry and Green, 1984)
178	44.88	45.11	22	8.94	14.54	
180	44.78	45.01	21.8	8.88	14.42	
185	44.52	44.75	21.65	8.85	14.34	
190	44.27	44.49	21.51	8.83	14.26	
200	43.74	43.96	21.21	8.77	14.1	
220	42.67	42.87	18.94	8.05	12.72	
250	40.96	41.14	18.12	7.91	12.29	
273.15						38.11
275	39.45	39.61	17.42	7.79	11.91	
300	37.83	37.97	16.69	7.66	11.53	
325	36.09	36.21	14.44	6.97	10.17	
337.15						35.23
350	34.20	34.29	12.93	6.55	9.29	
373.15						32.35
400	29.78	29.82	9.98	5.74	7.56	
433.125						25.94
450	23.87	23.36	8.47	5.46	6.75	
473.15						19.87
493.15						14.73
500	13.04	12.97	6.54	5.02	5.67	
513.15						0

Table A13-3. Heat of vaporization for **methanol** by 3 different methods as a function of temperature

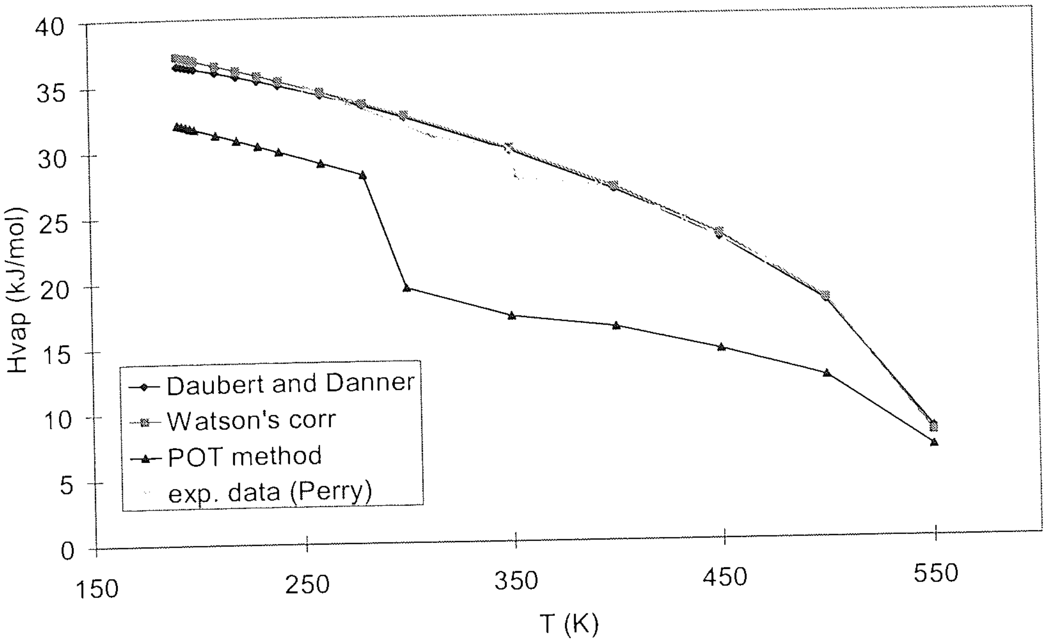

Figure A13.1. Heat of vaporization for **carbon tetrachloride**.

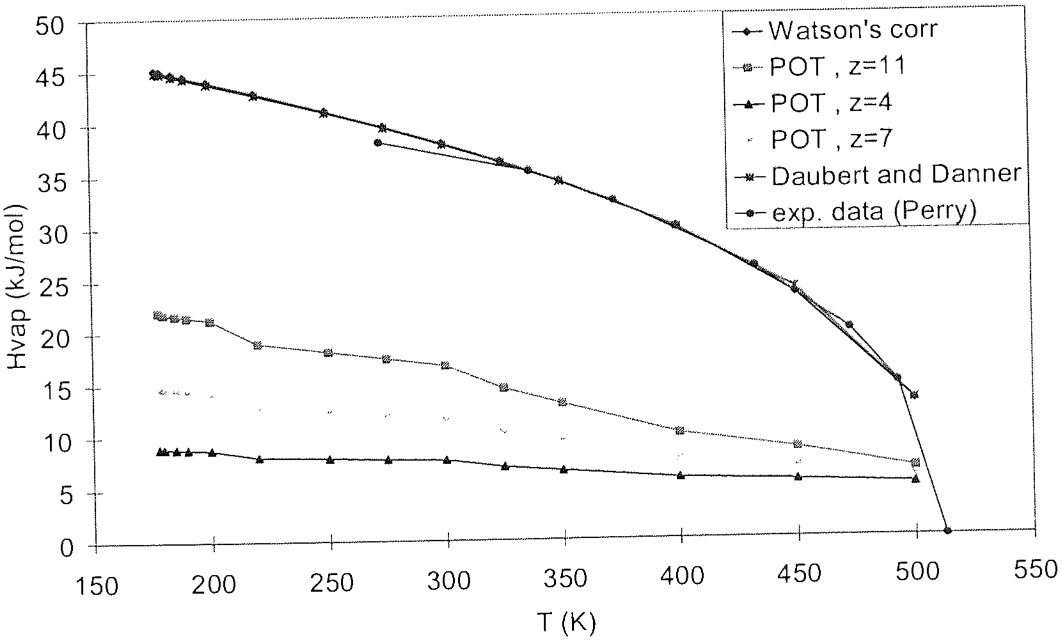

Figure A13.2. Heat of vaporization for **methanol**.

T (K)	Hvap (kJ/mol), method by Daubert and Danner (1984)	Hvap (kJ/mol) Watson's correlation	Hvap (kJ/mol) GLP , z=11	Hvap (kJ/mol) GLP , z=4	Hvap (kJ/mol) GLP , z=7	Hvap (kJ/mol) exp. data (Reid et al., 1987)
160	47.19	52.08	80.23	30.02	51.54	
162	47.19	51.96	79.54	29.78	51.1	
164	47.18	51.85	79.28	29.7	50.94	
166	47.18	51.74	79.01	29.61	50.78	
168	47.17	51.63	78.68	29.5	50.58	
170	47.16	51.51	78	29.26	50.15	
175	47.13	51.23	75.88	28.52	48.81	
180	47.09	50.94	74.75	28.13	48.11	
185	47.04	50.65	73.7	27.54	47.46	
190	46.98	50.35	71.6	27.04	46.14	
200	46.84	49.76	68.89	26.11	44.44	
220	46.45	48.53	64.38	24.57	41.63	
240	45.89	47.24	58.34	22.48	37.85	
260	45.16	45.9	53.06	20.67	34.55	
280	44.25	44.49	47.92	18.91	31.34	
300	43.13	43.01	42.69	17.11	28.07	
317						41.84
320	41.81	41.43	38.65	15.75	25.56	
340	40.26	39.75	33.67	14.04	22.45	39.75
360	38.46	37.95	29.45	12.61	19.83	37.66
380	36.38	36	25.82	11.4	17.58	35.56
400	34.01	33.85	21.85	10.06	15.11	
405						33.47
425						31.38
450	26.41	27.17	0	7.68	10.63	27.2
470						23.01
490						18.83
495						16.14
500	13.91	15.22	0	5.66	6.79	
505						12.55
510						9.41
517						0

Table A13-4. Heat of vaporization for **ethanol** by 3 different methods as a function of temperature. Experimental data from Reid et al (1987).

T (K)	Hvap (kJ/mol), method by Daubert and Danner (1984)	Hvap (kJ/mol) Watson's correlation	Hvap (kJ/mol) GLP , z=11	Hvap (kJ/mol) GLP , z=4	Hvap (kJ/mol) GLP , z=7	Hvap (kJ/mol) exp. data (Perry and Green, 1984)
180	36.81	36.67	109	40.59	69.91	
185	36.57	36.46	106.44	39.69	68.3	
190	36.33	36.24	105.48	39.36	67.7	
195	36.1	36.02	102.96	38.47	66.11	
200	35.86	35.8	102.01	38.15	65.52	
220	34.95	34.9	92.98	34.97	59.83	
240	34.05	33.96	85.05	32.2	54.85	
260	33.15	32.97	75.71	28.91	48.96	
273.15						32.76
280	32.24	31.94	66.56	25.68	43.2	
293.15						32.02
300	31.29	30.84	59.78	23.33	38.95	
313.15						31.12
333.15						30.01
350	28.62	27.78	41.13	16.81	27.23	
353.15						28.74
373.15						27.4
400	25.13	24.05	28.29	12.4	19.21	
450	19.9	18.99	17.18	8.63	12.29	
500	8.89	8.98	8.04	5.57	6.63	
508.15						0

Table A13-5. Heat of vaporization for **acetone** by 3 different methods as a function of temperature

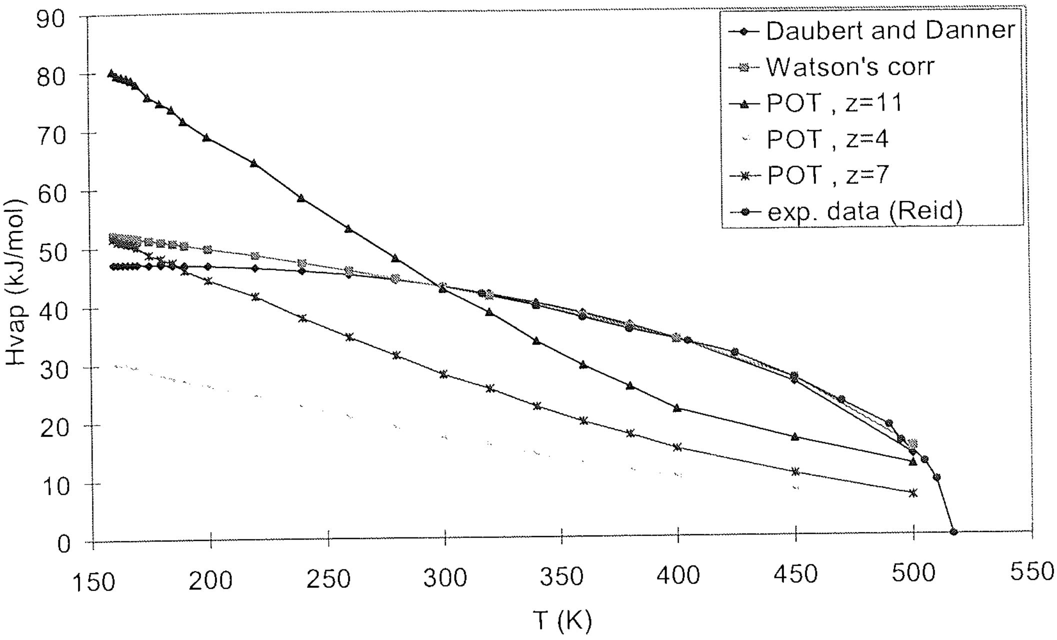

Figure A13.3. Heat of vaporization for **ethanol**.

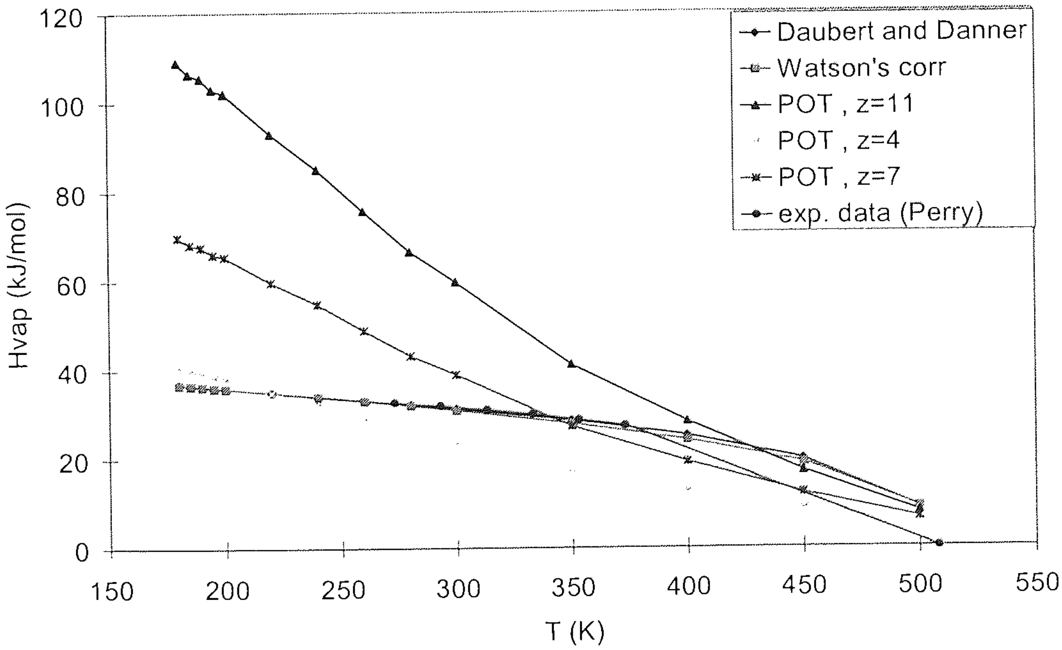

Figure A13.4. Heat of vaporization for **acetone**.

T (K)	Hvap (kJ/mol), method by Daubert and Danner (1984)	Hvap (kJ/mol) Watson's correlation	Hvap (kJ/mol) GLP , z=11	Hvap (kJ/mol) GLP , z=4	Hvap (kJ/mol) GLP , z=7	Hvap (kJ/mol) exp. data (Perry and Green, 1984)
290	21.65	28.41	51.74	20.35	33.8	
292	21.71	28.34	50.72	19.99	33.16	
294	21.77	28.27	50.2	19.81	32.84	
296	21.82	28.19	49.97	19.74	32.69	
298	21.88	28.12	49.79	19.68	32.59	
300	21.93	28.05	48.61	19.26	31.84	
320	22.43	27.3	43.51	17.51	28.65	
340	22.85	26.53	39.45	16.14	26.13	
360	23.15	25.71	35.64	14.87	23.77	
380	23.31	24.84	33.05	14.03	22.18	
391.45						24.31
400	23.31	23.93	29.51	12.85	19.99	
413.15						23.76
450	22.39	21.35	22.19	10.45	15.48	
493.15						20.41
500	19.82	18.12	16.47	8.63	11.99	
550	15.07	13.5	11.78	7.19	9.16	
590	8	4.73	7.19	5.74	6.36	
594.15						0

Table A13-6. Heat of vaporization for **acetic acid** by 3 different methods as a function of temperature

T (K)	Hvap (kJ/mol), method by Daubert and Danner (1984)	Hvap (kJ/mol) Watson's correlation	Hvap (kJ/mol) POT method	Hvap (kJ/mol) exp. data (Perry and Green, 1984)
280	34.75	34.49	41.07	
293.15				34.29
298.15				33.85
300	33.69	33.54	38.15	
313.15				32.66
320	32.61	32.54	35.34	
350	30.93	30.94	31.33	
353.2				30.77
393.15				28.41
400	27.88	27.94	22.53	
433.15				25.8
450	24.27	24.29	18.38	
473.15				22.21
500	19.42	19.4	12.33	
513.15				16.98
550	10.24	10.42	8.73	
553.15				9.14

Table A13-7. Heat of vaporization for **benzene** by 3 different methods as a function of temperature.

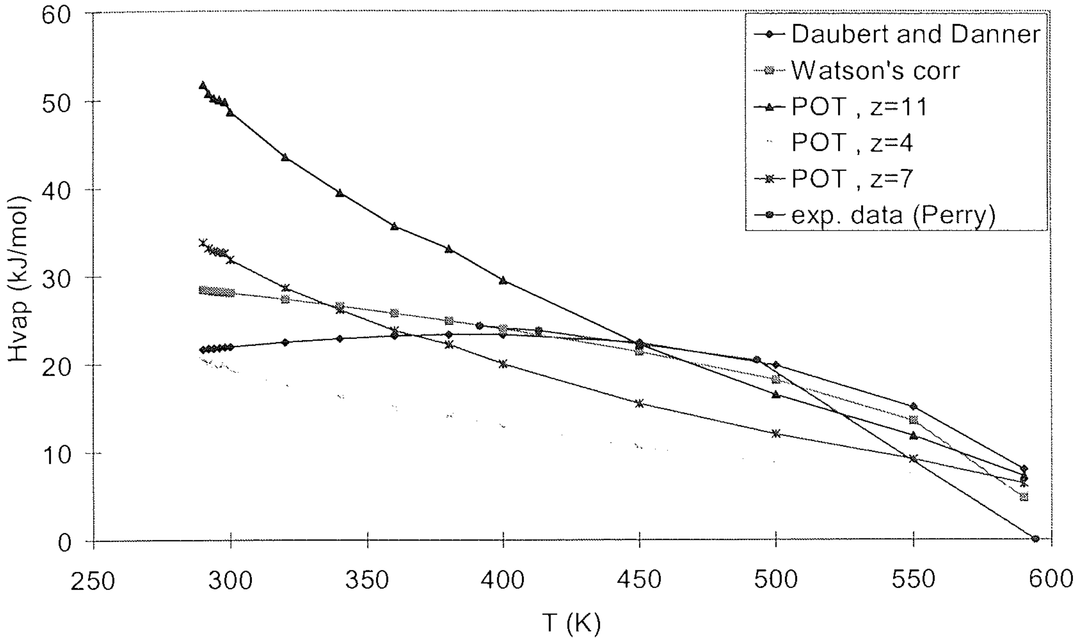

Figure A13.5. Heat of vaporization for **acetic acid**.

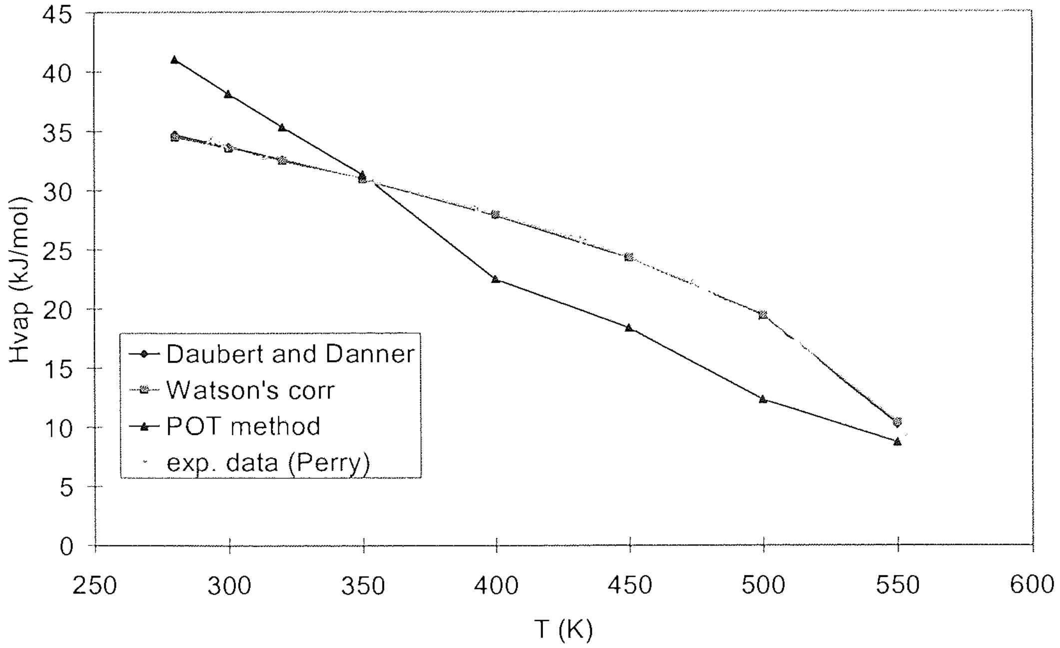

Figure A13.6. Heat of vaporization for **benzene**.

T (K)	Hvap (kJ/mol) Daubert and Danner (1984) method	Hvap (kJ/mol) Watson's corr	Hvap (kJ/mol) POT method	Hvap (kJ/mol) exp. data (Perry and Green, 1984)
55	7.72	8.05	4.21	
60	7.63	7.89	4.15	
63.15				7.49
70	7.41	7.56	4.03	
73.15				7.22
80	7.15	7.21	3.89	
83.15				7.09
90	6.83	6.83	3.75	
93.15				6.82
100	6.46	6.41	3.58	
103.15				6.29
113.15				6.02
120	5.5	5.39	3.2	
123.15				5.62
133.15				4.68
140	4.06	3.88	2.69	
143.15				3.61
150	2.75	2.5	2.28	
153.15				1.74

Table A13-8. Heat of vaporization for **oxygen** by 3 different methods as a function of temperature.

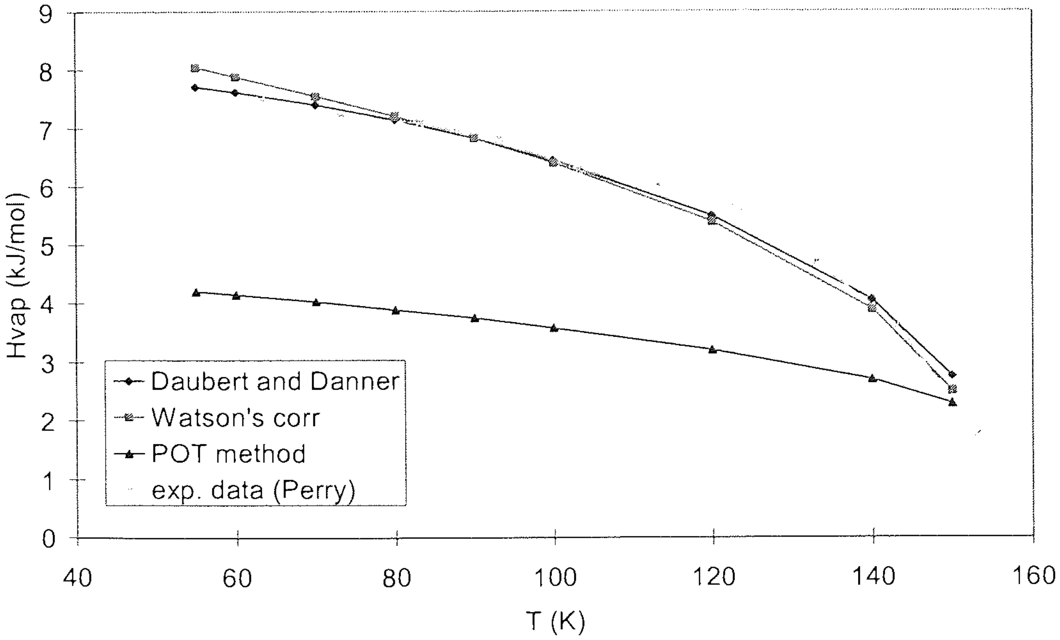

Figure A13.7. Heat of vaporization for **oxygen**.

T (K)	Hvap (kJ/mol), method by Daubert and Danner (1984)	Hvap (kJ/mol) Watson's correlation	Hvap (kJ/mol) POT method	Hvap (kJ/mol) exp. data (Perry and Green, 1984)
65	5.99	6.08	3.69	
70	5.82	5.88	3.69	
73.15				5.65
75	5.63	5.68	3.59	
77.35				5.59
80	5.44	5.46	3.48	
83.15				5.27
90	5.02	4.98	3.25	
93.15				4.92
100	4.49	4.4	2.98	
103.15				4.45
113.15				3.51
123.15				1.39
125	1.28	1.36	1.83	

Table A13-9. Heat of vaporization for **nitrogen** by 3 different methods as a function of temperature.

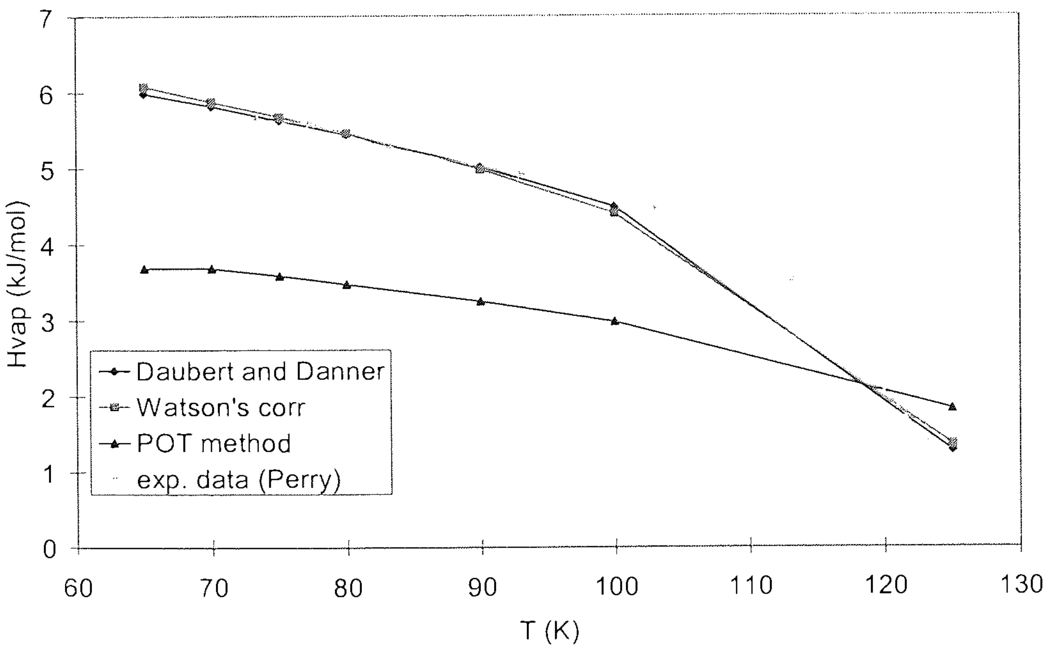

Figure A13.8. Heat of vaporization for **nitrogen**.

Appendix 14 - Results of molar volume calculations

A14.1 Introduction

The theoretical basis for the AGAPE theory has been described in section 2.11. The calculations use either the heat of vaporization or the molar volume to calculate the equilibrium separation for the pure compounds at the actual temperature. The equilibrium separation is a crucial parameter in the AGAPE calculations, mainly because it is occurs raised to the power of -6, thus an inaccurate equilibrium separation creates even greater errors in the final results.

It is therefore important to investigate how correct, the chosen methods for obtaining the heat of vaporization and the molar volume are. The heat of vaporization was examined in the previous Appendix, the molar volume in this Appendix. Both methods are extrapolated beyond the original areas of applicability.

A14.2 The Yen-Woods (1966) method for calculating the molar volume

The reduced saturated density ρ^S_r is given by

$$\rho_r^S = \frac{\rho^S}{\rho_C} = 1 + A(1 - T_r)^{1/3} + B(1 - T_r)^{2/3} + C(1 - T_r)^{4/3} \tag{A14.1}$$

where ρ_C is the density at the critical temperature and A, B, and C are functions of the critical compressibility factor Z_C (Yen and Woods, 1966), as follows

$$\begin{aligned}
A &= 17.44525 - 214.578\,Z_C + 989.825\,Z_C^2 - 1522.06\,Z_C^3 \\
B &= -3.28257 + 13.6377\,Z_C + 107.4844\,Z_C^2 - 384.21\,Z_C^3, \text{if } Z_C \leq 0.26 \\
B &= 60.2091 - 402.063\,Z_C + 501.0\,Z_C^2 + 641.0\,Z_C^3, \text{if } Z_C > 0.26 \\
C &= 0.93 - B
\end{aligned} \tag{A14.2}$$

The molar volume is then given by

$$v = R\ Z_C\ T_C\ /\ (P_C\ \rho^S) \tag{A14.3}$$

where R is the gas constant.

The observations made by Mohammadi (1986) were made based on the one of a modified pair potential at a standard temperature, where the like or the unlike pair potential is calculated at this temperature. The standard temperature used is in most cases the freezing temperature of the pure compound.

An investigation into how far the Yen-Woods method for calculating the molar volume can be used for compounds in their solid state is useful. The Yen-Woods method was designed for calculating the density of liquids in their liquid state and they obtained accurate results compared with experimental data (Yen and Wood, 1966).

A14.3 Results of the molar volume calculations

A14.3.1 Calculations at freezing points

Table A14-1 shows the results of the calculations.

The first column shows the name of the component and the second column displays the (normal) freezing points (from Reid et al. (1987)). The three next columns are the results obtained by running the PP program with the component and its freezing point as input to the program (which is described in section 2.11) and the modification PPT, both using the molar volume option. The molar volume is in the third column, then the equilibrium separation, then the like pair potentials. Next three columns are results obtained by running the same programs, but this time using the heat of vaporization option. The equilibrium separation is showed in the sixth column. From this equilibrium separation the equivalent molar volume has been calculated using the equation

$$v\ (\text{cm}^3/\text{mol}) = 0.4429\ (R^{A})^3 \qquad \text{(A14.4)}$$

provided R^{A} is in E-10 m (Å) and v in cm^3/mol. The constant 0.4429 takes into the account the Avogadro's number and the conversion factors. The seventh column shows the like pair potentials calculated by the heat of vaporization option.

The last two columns are from Mohammadi (1986). The first displays the molar volume as used by Mohammadi. The last column shows the experimental values of the equilibrium separation, again as used by Mohammadi.

compo-nent	freezing point (K)	AGAPE molar volume (cm^3/mol) program PP	AGAPE R^A (E-10 m) program PP molar vol.	AGAPE P (E-19 J) program PP molar vol.	AGAPE R^A (E-10 m) program PPT heat of vap.	AGAPE molar vol. (cm^3/mol) heat of vap.	AGAPE P (E-19 J) program PPT heat of vap.	Mohammadi's molar volume (cm^3/mol) (1986)	Mohammadi's R^A (e-10 m) experimental (1986)
Ne	24.5	16.32	3.32735	-0.00298077	2.940898	14.42452864	-0.006252	14	3.16
Ar	83.8	28.23	3.99434	-0.0125406	3.570308	25.23315362	-0.02459	24.12	3.76
Kr	115.8	34.06	4.25229	-0.0175001	3.961995	31.73479459	-0.026748	27.9	3.99
Xe	161.3	43.99	4.63092	-0.0238821	4.3316	41.14670174	-0.03566	36.76	4.33
H_2	14	24.06	3.78706	-0.00363868	3.943033	25.05092974	-0.002833	23.31	3.78
H_2O	273.15	17.48	3.40434	-0.0319748	2.845409	14.61010044	-0.131249	19.82	2.82
CH_4	90.7	35.09	4.29477	-0.0234382	4.262715	34.82809774	-0.024757	30.94	4.17
CS_2	161.3	57.75	5.07036	-0.122739	5.233804	59.61158202	-0.09424	61	
CCl_4	250	93.13	5.94618	-0.0876462	5.866148	91.87652631	-0.098824	87.9	5.9
C_6H_6	278.7	89.4	5.8656	-0.135591	6.019722	91.74903621	-0.097326	77.28	
c-C_6H_{12}	279.6	107.73	6.24186	-0.106143	6.305503	108.8284323	-0.094898	109.4	6.2
$C(CH_3)_4$	143.4	95.4	5.99408	-0.110448	6.153908	97.94377506	-0.084388	131.42	6.21
N_2	63.3	32.76	4.19743	-0.0107958	3.904841	30.47640846	-0.016954		
O_2	54.4	24.89	3.8303	-0.0137249	3.53888	22.99629878	-0.022979		
CO_2	216.6	37.61	4.3951	-0.0230543	4.042239	34.59047776	-0.04213		
C_2H_4	104	42.75	4.58674	-0.0512071	4.644384	43.28726198	-0.045998		
C_2H_6	89.9	48.55	4.78561	-0.0548896	4.80408	48.7373781	-0.053075		
CO	68.1	34.26	4.2604	-0.0111457	3.941879	31.69861387	-0.01824		
$SiCl_4$	204.3	113.85	6.35796	-0.106416	6.416656	114.9010509	-0.096797		

Table A14-1. Molar volumes, equilibrium separations, like pair of potentials calculated using the AGAPE computer programs and some values from Mohammadi (1986) (continued over).

component	freezing point (K)	AGAPE molar volume (cm^3/mol) program PP	AGAPE R^A (E-10 m) program PP molar vol.	AGAPE P (E-19 J) program PP molar vol.	AGAPE R^A (E-10 m) program PPT heat of vap.	AGAPE molar vol. (cm^3/mol) heat of vap.	AGAPE P (E-19 J) program PPT heat of vap.	Mohammadi's molar volume (cm^3/mol) (1986)	Mohammadi's R^A (e-10 m) experimental (1986)
$CHCl_3$	209.6	84.39	5.75392	-0.0665195	5.479028	80.35829016	-0.102302		
CH_2Cl_2	178.1	59.51	5.1213	-0.128902	5.247657	60.97828053	-0.098485		
CF_4	86.4	45.41	4.68033	-0.0304424	4.50533	43.71209622	-0.042189		
n-C_6H_{14}	177.8	114.35	6.36717	-0.14065	6.518808	117.0733143	-0.10881		
1,1-$C_2H_4Cl_2$	176.2	74.92	5.53013	-0.140957	5.348109	72.45405194	-0.210682		
1,2-$C_2H_4Cl_2$	237.5	71.71	5.44986	-0.231646	5.467603	71.94346481	-0.221777		
C_2HCl_3	186.6	79.5	5.64052	-0.271999	5.707529	80.44445468	-0.231606		
CH_3OH	175.6	34.63	4.27597	-0.0714642	4.023908	32.58861359	-0.132165		
C_2H_5OH	159.1	48.48	4.78321	-0.25358	4.97299	50.40350626	-0.15335		
CHF_3	110	40.79	4.51573	-0.0434629	4.352645	39.31687447	-0.05981		
n-C_3H_8	85.5	63.99	5.24683	-0.0945361	5.386187	65.68958898	-0.072307		
n-C_4H_{10}	134.8	79.97	5.65164	-0.146552	5.923813	83.82121395	-0.082965		
Cl_2	172.2	42.12	4.56415	-0.0544741	4.45336	41.09758075	-0.065202		
Br_2	266	41.94	4.55775	-0.135175	4.785632	44.03694939	-0.092721		
c-C_5H_{10}	179.3	84.61	5.75898	-0.106739	5.81186	85.38690438	-0.097543		

Table A14-1. Molar volumes, equilibrium separations, like pair of potentials calculated using the AGAPE computer programs and some values from Mohammadi (1986).

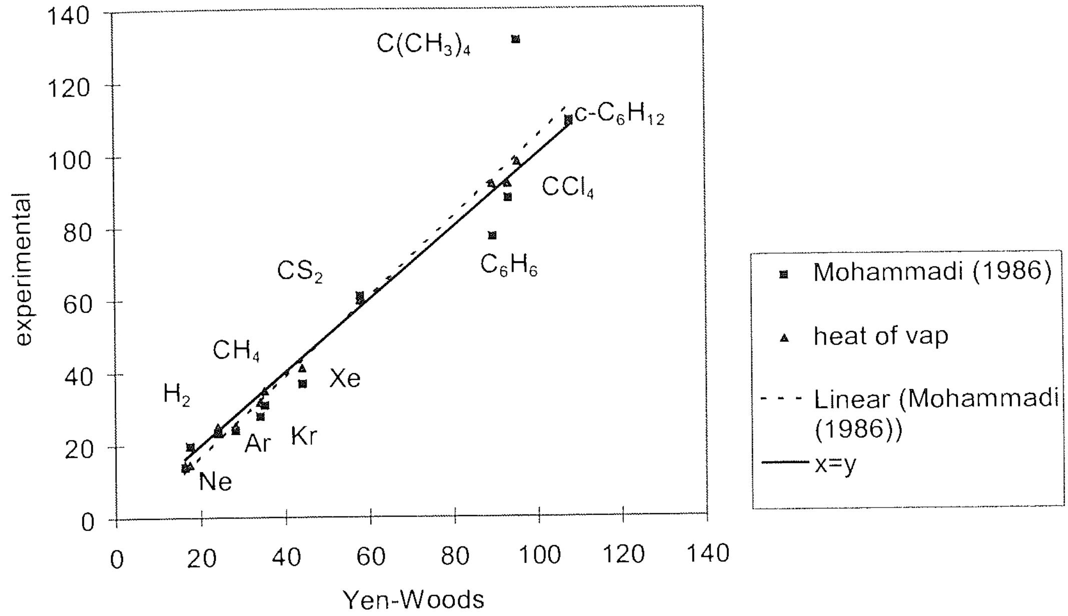

Figure A14.1. The molar volume (cm^3/mol) as used by Mohammadi (1986) (y-axis -- best fitted line and ■ points), the molar volume (cm^3/mol) calculated by the GLP method using the heat of vaporization option (▲ points) and the molar volume (cm^3/mol) calculated by the Yen-Woods (1966) method (x-axis) at the components freezing points.

In Figure A14.1 solid line represents the x equals y and the dotted line the best fitted line through the ■ points. Figure A14.1 shows the result of a comparison for the molar volume. The solid molar volume calculated by the Yen-Woods method is plotted against the experimental solid molar volume as given in Mohammadi (1986).

Figure A14.2 shows the equilibrium separation as calculated by the AGAPE method (employing the Yen-Woods for the molar volumes) versus the experimental equilibrium separation as given in Mohammadi (1986). In Figure A14.2 the solid line represents the x equals y and the dotted line the best fitted line through the ■ points.

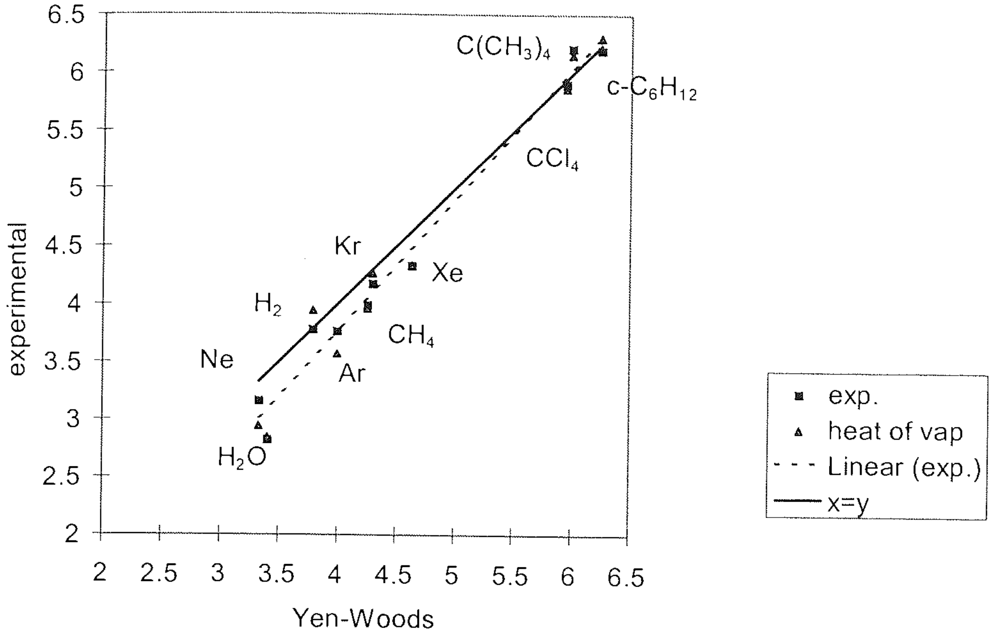

Figure A14.2. The equilibrium separation (10^{-10} m) as used by Mohammadi (1986) (y-axis, -- best fitted line and ■ points), the equilibrium separation (10^{-10} m) calculated by the GLP method using the heat of vaporization option (▲ points) and the equilibrium separation (10^{-10} m) as calculated by the Yen-Woods (1966) method (x-axis) at the components freezing points.

Table A14-2 shows the same as Table A14-1. The first column shows the name of the component and the second column displays a temperature from Homer and Mohammadi (1987b)). The next column shows the results obtained by running the PP program (which is described in section 2.11) at the actual temperature in column 2 using the molar volume option. The molar volume is in the third column. The fourth column displays the molar volume from Homer and Mohammadi (1987b) at the temperatures in column 2. The fifth column shows the equilibrium separation at the temperatures in column 2 calculated using the computer program PP. The last column is from Homer and Mohammadi (1987b) and displays the equilibrium separation at the temperature in column 2.

Component	Temperature from Mohammadi and Homer (1987b) (K)	AGAPE molar volume (cm^3/mol) at Mohammadi's temperature. Program PP	Homer and Mohammadi's molar vol. (cm^3/mol) (1987b)	AGAPE program PP R^A (E-10 m) at Mohammadi's temperature	Homer and Mohammadi's R^A (E-10 m) (1987b)
CH_4	109.7	37	34.42	4.37109	4.27
CS_2	293.15	63.65	60.38	5.23756	5.14
c-C_6H_{12}	293.15	109.32	108.09	6.2725	6.25
N_2	77.65	34.91	34.67	4.2872	4.28
O_2	20.65	23.08	22.43	3.73475	3.7
CO_2	194.15	35.43	28.2	4.30842	3.99
C_2H_4	171.15	48.81	49.56	4.794	4.82
C_2H_6	165.15	54.58	52.57	4.97592	4.91
CO	78.15	35.64	34.73	4.31695	4.28
$SiCl_4$	303.15	125.77	114.55	6.57251	6.37
$CHCl_3$	303.15	91.49	81.1	5.91101	5.67
CH_2Cl_2	303.15	68.25	64.9	5.36092	5.27
CF_4	89.15	45.69	44.89	4.6896	4.66
n-C_3H_8	228.15	77.91	75.6	5.6028	5.55
n-C_4H_{10}	273.15	96.49	96.69	6.01677	6.02
Cl_2	172.2	41.13	34.75	4.52801	4.28
Br_2	293.15	43.06	57.2	4.59798	4.87
c-C_5H_{10}	293.15	95.62	94.01	5.99863	5.96

Table A14-2. Molar volumes, equilibrium separations, like pair of potentials calculated using the AGAPE computer programs and some values from Homer and Mohammadi (1987b).

The molar volume and the equilibrium separation have both been plotted. Figures A14.3 and A14.4 show the plots.

In Figure A14.3 the solid line represents the x equals y and the dotted line the best fitted line through the points.

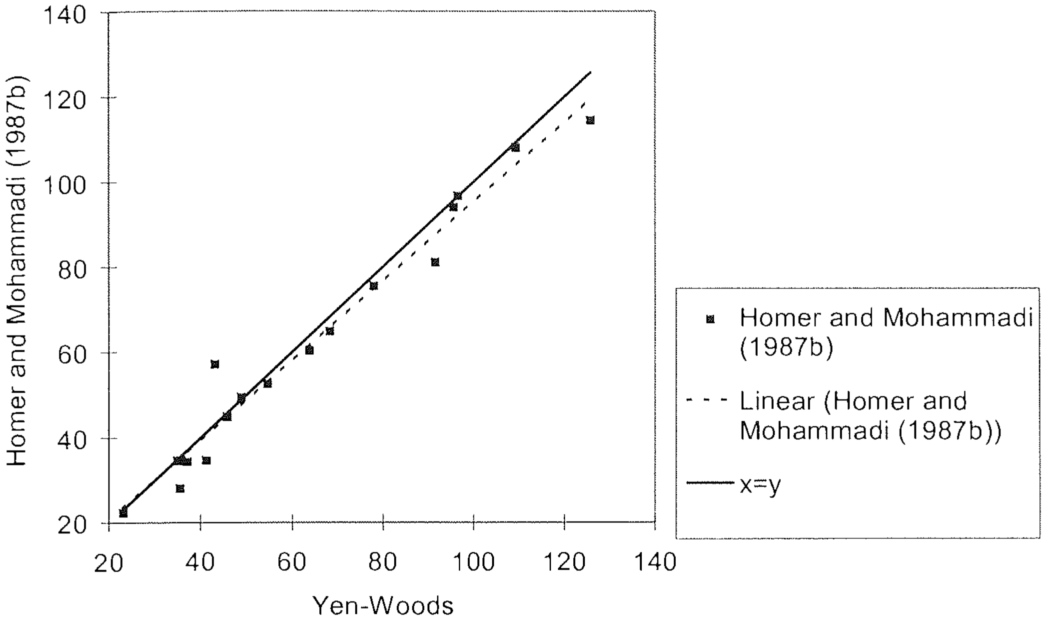

Figure A14.3. The molar volume (cm^3/mol) as used by Homer and Mohammadi (1987b) (y-axis, -- best fitted line and ■ points) and the molar volume (cm^3/mol) as calculated by the Yen-Woods (1966) method (x-axis) at the component's freezing points.

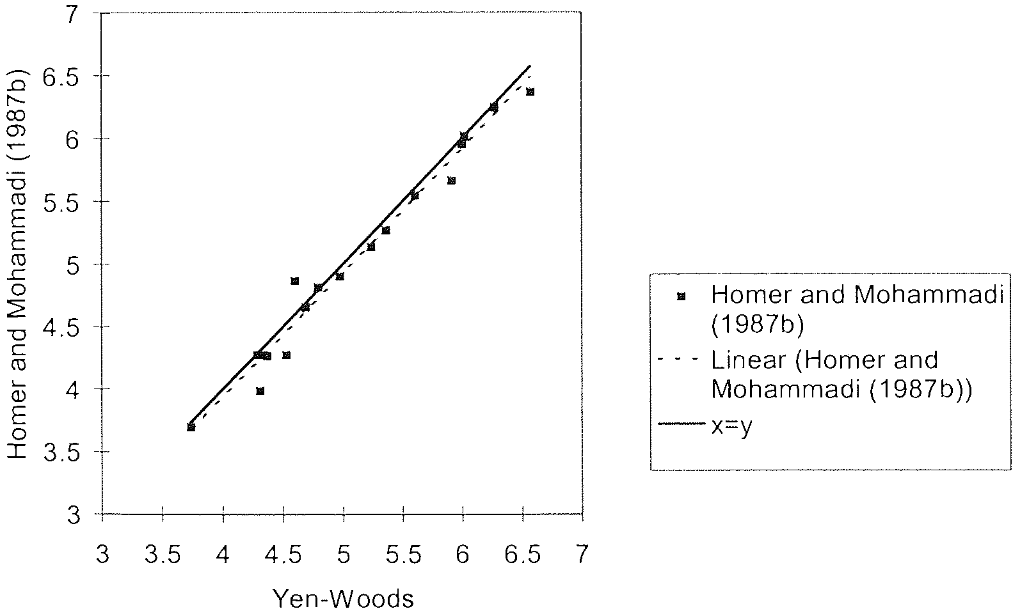

Figure A14.4. The equilibrium separation (10^{-10} m) as used by Homer and Mohammadi (1987b) (y-axis, -- best fitted line and ■ points) and the equilibrium separation (10^{-10} m) as calculated by the Yen-Woods (1966) method (x-axis) at the temperatures in Table A14-2.

In Figure A14.4 one line represents the x equals y and the other the best fitted line through the points.

All the previous calculations carried out show that the unlike London pair potential is very sensitive to the equilibrium separation. A comparison between the experimental equilibrium separations for a series of compounds and the equilibrium separations obtained from both the molar volume and the heat of vaporization will show which option gives the most accurate results.

Figures A14.5and A14.6 show the results of the comparison. The like London pair potential for the pure compound has been calculated for nearly all the compounds in the AGAPE database at their melting points. For every compound two like London pair potentials have been calculated, one from the molar volume option, the other from the heat of vaporization. The calculations also give the equilibrium separations, again two values from the two options. The data in Figures A14.5 and A14.6 have not been labelled as this will clutter up the graphs. Figure A14.6 shows the equilibrium separations calculated using the two options at the component's freezing points.

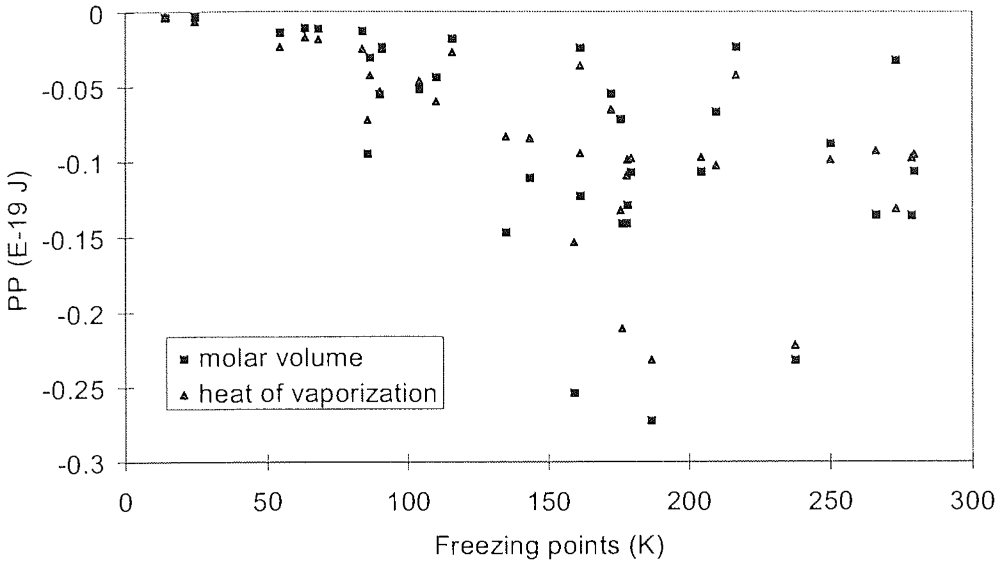

Figure A14.5. The like pair potentials (obtained from both the heat of vaporization and the molar volume option) for the compounds in Table A14-1 as a function of the component's freezing points.

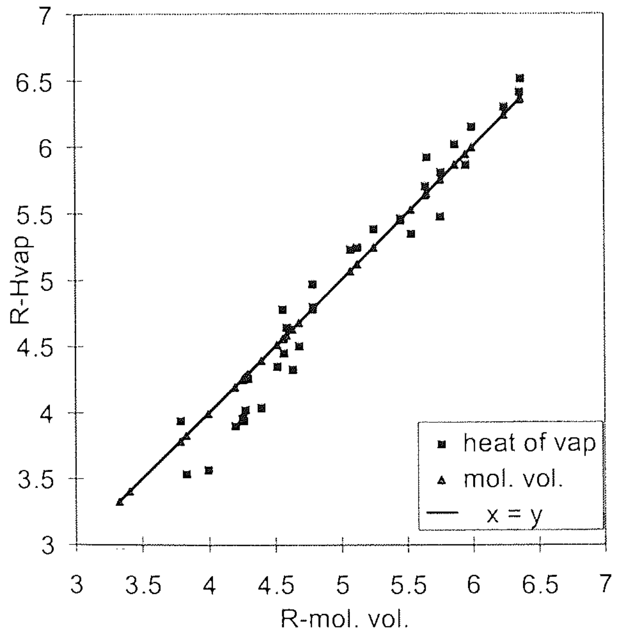

Figure A14.6. The R^A molar volume option (10^{-10} m) along the x-axis and the heat of vaporization R^A values (10^{-10} m) as the points.

The figures show that the like London pair potential is very sensitive to the value of the equilibrium separation.

A14.3.2 Calculations at 298.15 K

Hildebrand et al. (1972) give values for the molar volume of the gaseous component as a hypothetical liquid at 298.15 K. These values are compared with the values of the molar volume that can be obtained from the equilibrium separation at 298.15 K using the extrapolation method described in section 4.4.

The majority of the gaseous components mentioned in Hildebrand et al. (1972) have critical temperatures lower then 298.15 K. The extrapolating method (described in section 4.4) has been applied to the components, and values of the equilibrium separation for each component at 298.15 K using both options of molar volume and heat of vaporization have been derived. These values can be used to calculate a value for the molar volume at 298.15 K for the relevant gases using equation (A14.4).

Table A14-3 shows the results of the calculations.

298.15 K compound	**heat of vaporization R^A (E-10 m)**	**v (cm3/mol) from heat of vaporization**	**molar volume R^A (E-10 m)**	**v (cm3/mol) from molar volume**	**v-hyp (cm^3/mol) Prausnitz et al. (1986)**
methane	4.99829	55.31820468	5.173	61.32409693	52
argon	4.784437	48.51725787	5.03754	56.63165441	57.1
nitrogen	5.32727	66.97579106	5.76097	84.70139581	32.4
oxygen	4.423303	38.33926617	4.883527	51.59463041	33
carbon dioxide	5.222152	63.08879784	5.625801	78.87816958	55
carbon monoxide	5.222174	63.08959519	5.62584	78.87981003	32.1
ethylene	5.029482	56.36032656	5.187144	61.82848998	65

Table A14-3. Molar liquid volumes for selected (hypothetical) gases and liquids at 298.15 K as calculated by the Yen-Woods method and values from Prausnitz et al. (1986).

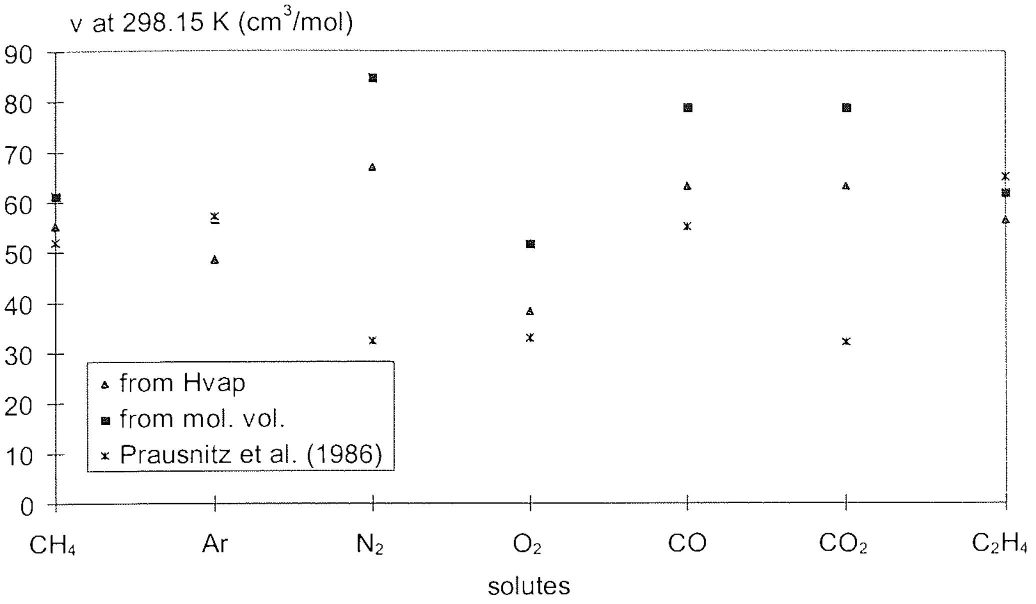

Figure A14.7. The molar volumes (cm^3/mol) from Table A14-3 plotted for each component.

Appendix 15 - Results of the MOSCED calculations

The results obtained of the calculations are shown in Table A15-1. The first column gives the chemical formulae of the component and then the name of the component follows. The third column displays the values of the molar volume (at 293.15 K) as stated in Thomas and Eckert (1984). The fourth column shows the MOSCED parameter λ (from Thomas and Eckert, 1984), which accounts for the dispersion forces in the MOSCED equations. Then follows the (natural) logarithm of λ. The three next columns are the results obtained by running the PP program with the component and the temperature 293.15 K as input to the program (which is described in section 2.11) using the molar volume option. The molar volume is in the sixth column, then the equilibrium separation, then the like pair of potentials. Next three columns are results obtained by running the same program this time using the heat of vaporization option. The heat of vaporization is showed in column ten, then follows the equilibrium separation and the like pair of potentials calculated by the heat of vaporization option.

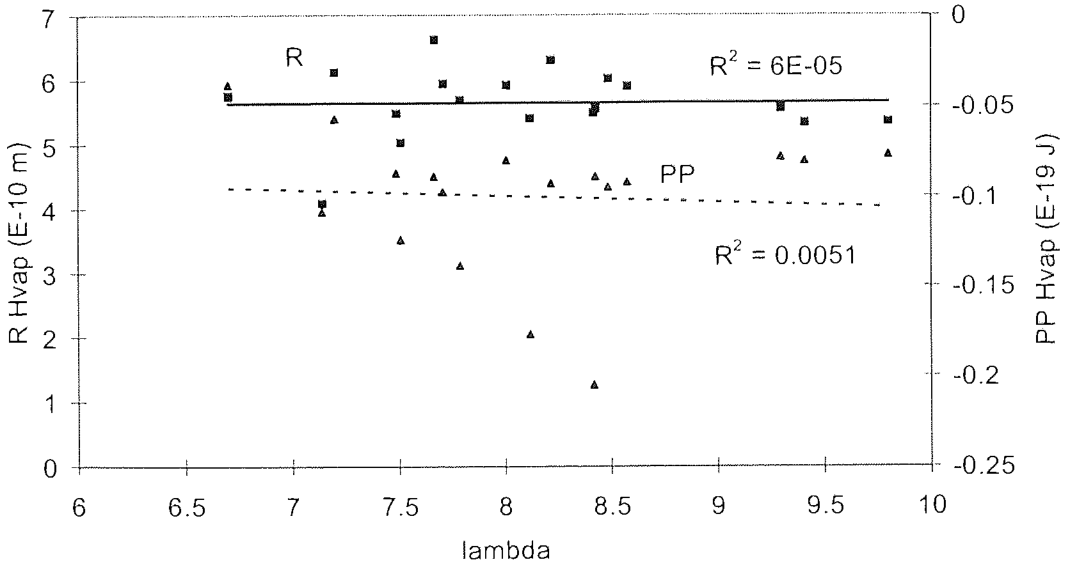

Figure A15.1. The equilibrium separation (■, left y-axis and – line) and the like pair potential (points ▲, right y-axis and -- line), both obtained from the heat of vaporization option as a function of λ and the best fitted straight lines.

component	name	v-MOSCED (cm^3/mol)	lambda-MOSCED λ	ln(lambda-MOSCED) ln (λ)	v-GLP (cm3/mol)	R^A-GLP (from mol. vol.) (E-10 m)	PP(Φ)-GLP (mol. vol) (E-19 J)	Hvap (J/mol)	R^A-GLP (Hvap) (E-10 m)	PP(Φ)-GLP (Hvap) (E-19 J)
CS_2	carbon disulfide	72.0	9.80	2.28	63.65	5.23756	-0.093687	27844.73	5.36857	-0.076694
CCl_4	carbon tetrachloride	96.5	8.58	2.15	97.39	6.03544	-0.076959	32886.48	5.914	-0.091943
$CHCl_3$	chloroform	80.7	8.43	2.13	90.57	5.89103	-0.054476	31873.45	5.56594	-0.088864
CH_2Cl_2	dichloro-methane	69.5	9.41	2.24	67.37	5.33767	-0.082285	29030.99	5.3502	-0.080316
CH_3OH	methanol	40.5	7.14	1.97	39.35	4.46188	-0.048268	38428.71	4.0991	-0.108678
CH_3I	methyl iodide	79.1	9.30	2.23	69.6	5.39604	-0.109699	28254.44	5.57324	-0.077948
1,2-$C_2H_4Cl_2$	1,2-dicloroethane	79.1	8.42	2.13	75.82	5.5521	-0.181625	70331.64	5.50081	-0.204738
1,1-$C_2H_4Cl_2$	1,1-dicloroethane	84.2	8.12	2.09	84.58	5.75826	-0.090274	60997.69	5.42526	-0.176812
C_2H_5OH	ethanol	58.4	7.51	2.02	55.83	5.01375	-0.13665	43526.25	5.04819	-0.124086
C_3H_6O	acetone	74.4	7.49	2.01	69.76	5.40016	-0.108019	31238.29	5.49698	-0.086911
C_3H_8	n-propane	88.1	6.70	1.90	90.79	5.89581	-0.031187	14985.88	5.76802	-0.037871
C_3H_7OH	1-propanol	74.8	7.79	2.05	73.17	5.48662	-0.209386	48267.17	5.705	-0.138381
C_4H_8O	butanone (MEK)	89.6	7.71	2.04	89.32	5.86378	-0.114013	34727.7	5.95449	-0.097438
n- C_4H_{10}	n-butane	100.4	7.20	1.97	100.15	6.09182	-0.061092	21208.28	6.13573	-0.056654
c-C_5H_{10}	*cyclo*-pentane	94.1	8.01	2.08	95.62	5.99863	-0.072074	28828.55	5.93491	-0.079708
C_6H_6	benzene	89.1	8.49	2.14	90.78	5.89561	-0.126781	33867.1	6.03242	-0.094846
c-C_6H_{12}	*cyclo*-hexane	108.1	8.22	2.11	109.32	6.2725	-0.100522	33141.22	6.31918	-0.09269
n-C_6H_{14}	n-hexane	130.8	7.67	2.04	130.12	6.64728	-0.086986	31836.51	6.636	-0.088729

Table A15-1. Values for the dispersion parameter in the MOSCED method and molar volumes, equilibrium distances, and like potentials calculated from the AGAPE method for selected pure compounds.

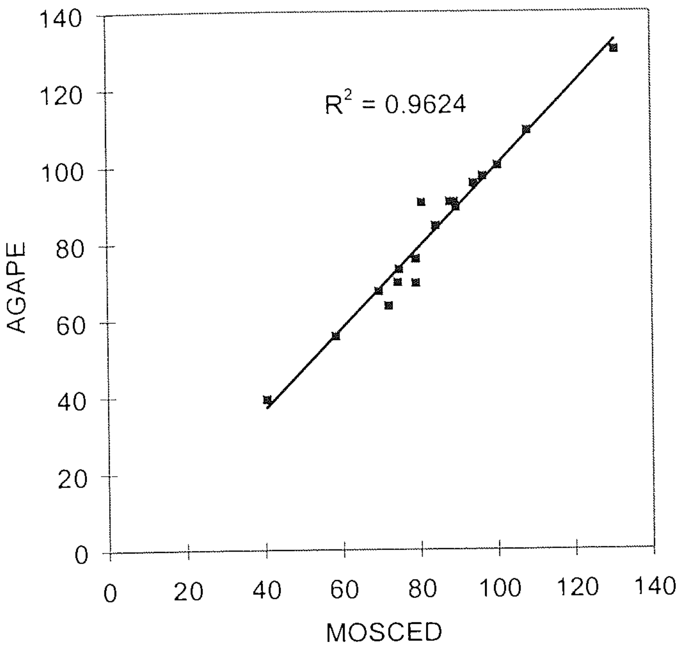

Figure A15.2. Molar volume as calculated by the Yen-Woods method (1966) as a function of the molar volume as stated by Thomas and Eckert (1984) and the best fitted straight line through the points.

Appendix 16 - Databank

A16.1 Databank for excess thermodynamic properties

To determine whether we can separate out the contributions from the different terms in the calculation of the Gibbs free energy, the experimental excess thermodynamic data for 45 binary mixtures have been collected. The activity coefficients, the excess Gibbs free energies, and the vapour pressures may be calculated from the AGAPE relationships.

The databank consist of spreadsheets of experimental data for each binary system. The intentions are then to use the AGAPE equations to calculate activity coefficients, Gibbs excess free energy and excess entropy for the systems under the same condition (temperature, mole fractions and pressure) as the experimental data. The experimental data and predicted results will then be compared.

There are a number of databanks available in the literature, but not one which contains the experimental excess thermodynamic properties for a number of binary mixtures.

The databank is for the experimental excess thermodynamic properties readily accessible in the literature, and contains mainly the excess entropy (S^E) and the excess volume (V^E) values, in addition to the excess enthalpy (H^E) and the excess Gibbs free energy (G^E), where possible. All properties are collected as a function of temperature, composition (mole fraction of gas or liquid) and pressure.

temperature, T (K)
liquid phase mole fraction, x_1 or x_2
vapour mole fraction, y_1 or y_2
total pressure, P (10^5 Pa)
temperature times excess entropy, $T*s^E$ (J/mol)
excess volume, v^E (cm^3/mol)
excess enthalpy, h^E (J/mol)
excess Gibbs free energy, g^E (J/mol)
heat capacity, C_P (J/mol/K)

activity coefficient of component 1, γ_1

activity coefficient of component 2, γ_2

The databank are for the 45 binary mixtures in Table A16-1. All the compounds are included in the AGAPE database, that means we can calculate VLE and excess Gibbs free energy for mixtures with these compounds. The mixtures appear to consist only of ideal or nearly ideal mixtures, but calculation of the activity coefficients (Homer et al., 1991) have showed that a number of the mixtures have activity coefficients far from 1.0.

A16.2 Thermodynamic data tables

1. N_2 - CO
2. CCl_4 - $c\text{-}C_5H_{10}$
3. N_2 - O_2
4. Ar - N_2
5. CO - CH_4
6. Ar - CO
7. CH_4 - C_2H_6
8. $SiCl_4$ - CCl_4
9. $c\text{-}C_6H_{12}$ - $C(CH_3)_4$ (neopentane)
10. N_2 - CH_4
11. CH_4 - $n\text{-}C_3H_8$
12. C_6H_6 - $c\text{-}C_5H_{10}$
13. CCl_4 - CH_2Cl_2
14. C_6H_6 - $C(CH_3)_4$ (neopentane)
15. $C(CH_3)_4$ (neopentane) - $Si(CH_3)_4$
16. $Si(CH_3)_4$ - $Sn(CH_3)_4$
17. CCl_4 - $TiCl_4$
18. CCl_4 - $SnCl_4$
19. $SiCl_4$ - $TiCl_4$
20. $SiCl_4$ - $SnCl_4$
21. $TiCl_4$ - $SnCl_4$
22. O_2 - Kr
23. C_6H_6 - $c\text{-}C_6H_{12}$
24. CCl_4 - $c\text{-}C_6H_{12}$
25. CS_2 - CCl_4
26. CS_2 - C_6H_6
27. $CHCl_3$ - CCl_4
28. C_6H_6 - CCl_4
29. CCl_4 - $C(CH_3)_4$ (neopentane)
30. CCl_4 - CH_3I
31. CH_3I - CH_2Cl_2
32. CH_3I - CH_3Cl
33. Ar - Kr
34. Ar - C_2H_4
35. Kr - C_2H_4
36. C_2H_6 - C_2H_4

Table A16-1. The mixtures included in the databank of excess properties. (continued over).

37. CH_4 - C_2H_4
38. Kr - Xe
39. Xe - C_2H_4
40. CI_4 - CH_4
41. Ar - O_2
42. Ar - CH_4
43. Xe - CI_4
44. Kr - C_2H_6
45. Xe - C_2H_6

Table A16-1. The mixtures included in the databank of excess properties.

The databank is available from the author on request.