Pressure and Temperature Dependence of Excess Enthalpies of Methanol + Tetraethylene Glycol Dimethyl Ether and Methanol + Polyethylene Glycol Dimethyl Ether 250

Enriqueta R. López,[†,‡] Jean-Yves Coxam,[†] Josefa Fernández,[‡] and Jean-Pierre E. Grolier*,[†]

Laboratoire de Thermodynamique et Génie Chimique (UPRES A 6003), Université Blaise-Pascal, F-63177 Aubière, France, and Laboratorio de Propiedades Termofísicas, Departamento de Física Aplicada, Universidad de Santiago, E-15706 Santiago de Compostela, Spain

The excess molar enthalpies at 323.15 K, 373.15 K, and 423.15 K, at 8 MPa, are reported for the binary mixtures methanol + tetraethylene glycol dimethyl ether (TEGDME) and methanol + poly(ethylene glycol) dimethyl ether 250 (PEGDME 250). Excess molar enthalpies were determined with a Setaram C-80 calorimeter equipped with a flow mixing cell. For both systems, the excess enthalpies are positive over the whole composition range, increasing with temperature. The $H^E(x)$ curves are slightly asymmetrical, and their maxima are skewed toward the methanol-rich region. The excess enthalpies slightly change with the pressure, the sign of this change being composition-dependent. In the case of mixtures with TEGDME, the experimental H^E values have been compared with those predicted with the Gmehling et al. version of UNIFAC (Dortmund) and the Nitta–Chao and DISQUAC group contribution models.

Introduction

The recent renaissance of absorption heat cycles, incorporated in different networks of thermal recovery systems, is a consequence of the potential impact on the ozone layer of chlorofluorinated carbons (CFC's) used until recently in a majority of mechanical heat pumps, and their subsequent contribution to the greenhouse effect. In the past years, several organic compounds have been proposed as working fluids of absorption machines in order to improve the characteristics of the classical working pairs (Nowaczyk and Steimle, 1992; Moncada et al., 1994).

Methanol as a refrigerant combined with polyglycol ethers as absorbents may be promising working pairs for high-temperature heat pump applications because their molecular structures meet a great number of prerequisites (Moncada et al., 1994). The refrigerant properties of the alcohols and their mixtures with other compounds are related to the hydrogen-bonding capability of the alcohols. In this context methanol has been proposed as a refrigerant. Moreover, methanol presents other important advantages such as a large value of latent heat and the faculty to reach evaporating temperature under 0 °C.

Polyglycol ethers are molecules that are thermally and chemically stable, with boiling points much higher than that of methanol and with high solubility in methanol. In addition, dimethyl ether functional groups present a strong affinity for small polar molecules such as methanol.

Absorption machine performance depends on the characteristics of the cycle and on the properties of the working mixtures. Up to now, Kuczynski et al. (1986) and Esteve et al. (1995a) have studied the vapor–liquid equilibria (VLE) of methanol with tetraethylene glycol dimethyl ether, and Herraiz et al. (1998) the VLE of methanol + poly(ethylene glycol) dimethyl ether 250. Esteve et al. (1994, 1995b) have also reported the excess viscosities and excess volumes for both mixtures. López et al. (1997), Esteve (1995), and Esteve et al. (1994) have measured the excess enthalpies and excess volumes of methanol–polyglycol ether mixtures at atmospheric pressure. Nevertheless, to determine the cycle performance, it is also necessary to know the enthalpic and volumetric properties of both the pure liquids and their mixtures as functions of pressure, temperature, and composition. This work reports the excess molar enthalpies H^E at 323.15, 373.15, and 423.15 K, at 8 MPa, of binary mixtures containing methanol and TEGDME (tetraethylene glycol dimethyl ether) or PEGDME 250 (poly(ethylene glycol) dimethyl ether).

Experimental Section

Materials. Methanol (Aldrich with purity > 0.999 mole fraction), TEGDME (Aldrich, with 0.99 mole fraction purity), and PEGDME 250 (Aldrich) were subjected to no further purification other than drying with Union Carbide 0.4 nm molecular sieves. PEGDME 250 is a mixture of poly(ethylene glycol) dimethyl ethers $CH_3O(CH_2CH_2O)_nCH_3$ where $n = 3-9$. The product used in the present study, analyzed by gas chromatography and mass spectrometry (López et al., 1997), had the molecular weight 279.55.

Apparatus. Excess enthalpies were determined with a modified Setaram C-80 calorimeter equipped with a flow mixing cell designed by Mathonat et al. (1994). The temperature of the fluids was regulated and controlled within ±0.05 K during the experiment. The required pressure was regulated to better than ±0.02 MPa. The performance of the apparatus was checked prior to actual measurements using the reference test mixture ethanol + water (Mathonat et al., 1994); the accuracy of the excess enthalpies was estimated to be better than 2%. Flow rates were selected to cover the whole mole fraction range. The

* To whom the correspondence should be addressed. E-mail: j-pierre.grolier@univ-bpclermont.fr.
[†] Université Blaise Pascal.
[‡] Universidad de Santiago.

Table 1. Experimental Excess Molar Enthalpies H^E for the Systems Methanol + TEGDME at 8 MPa and at 323.15 K, 373.15 K, and 423.15 K

x	$H^E/\text{J·mol}^{-1}$	x	$H^E/\text{J·mol}^{-1}$	x	$H^E/\text{J·mol}^{-1}$	x	$H^E/\text{J·mol}^{-1}$
			$T = 323.15$ K				
0.0686	134.9	0.3500	538.0	0.5091	616.5	0.7538	481.6
0.1000	193.3	0.4022	588.1	0.5608	614.0	0.7977	418.8
0.1441	273.5	0.4023	577.6	0.6056	604.6	0.8550	312.2
0.1849	336.1	0.4699	605.6	0.6567	586.0	0.8988	220.4
0.2227	392.5	0.4700	611.3	0.7000	548.7	0.9333	141.3
0.2907	478.7						
			$T = 373.15$ K				
0.0686	163.3	0.2909	611.0	0.5093	791.8	0.7540	643.2
0.1001	242.5	0.3502	690.9	0.5610	797.9	0.7978	564.8
0.1442	348.6	0.4024	734.0	0.6058	787.0	0.8551	430.5
0.1850	431.3	0.4025	744.3	0.6569	755.7	0.8989	310.8
0.2229	499.3	0.4701	779.5	0.7002	715.5	0.9334	205.7
			$T = 423.15$ K				
0.0686	196.2	0.3502	752.5	0.5092	877.9	0.7002	811.8
0.1001	279.1	0.3502	758.3	0.5610	899.4	0.7539	707.0
0.1442	382.6	0.4024	806.2	0.6057	894.8	0.7977	616.3
0.1850	468.9	0.4024	812.3	0.6568	871.2	0.8449	485.2
0.2229	545.3	0.4024	820.9	0.6991	820.0	0.8989	322.7
0.2909	668.0	0.4700	861.7	0.7001	837.0	0.9334	210.5

volumetric flow rates were converted to mass flow rates and to mole fractions using the densities of the components at the temperature of the circulating pumps, at 8.0 MPa. For this reason, the pressure dependent densities for methanol, TEGDME, and PEGDME 250 were calculated using the Tait equation in the following form proposed by Cibulka and Ziková (1994):

$$\rho(T,P,\bar{c},\bar{b}) = \frac{\rho(T,P_{\text{ref}}(T))}{1 - C(T,\bar{c}) \ln\left(\frac{(B(T,\bar{b}) + P)}{B(T,\bar{b}) + P_{\text{ref}}(T)}\right)} \quad (1)$$

where $\rho(T,P_{\text{ref}}(T))$ gives the temperature dependence of the density at the reference pressure ($P_{\text{ref}} = 101.3$ kPa). The following polynomial expression for $\rho(T,P_{\text{ref}}(T))$ has been used:

$$\rho(T,P_{\text{ref}}(T)) = \sum_{i=0}^{N} A_i (T/100)^i \quad (2)$$

The denominator of eq 1 changes with both temperature and pressure, through $C(T,\bar{c})$ and $B(T,\bar{b})$ which have also been expressed by the following polynomial functions:

$$C(T,\bar{c}) = \sum_{i=0}^{Nc} c_i [(T - T_0)/100]^i \quad (3)$$

$$B(T,\bar{b}) = \sum_{i=0}^{N_B} b_i [(T - T_0)/100]^i \quad (4)$$

For methanol we have taken $C(T,\bar{c})$ and $B(T,\bar{b})$ from Cibulka and Ziková (1994) whereas the parameters of eq 2 were determined in this work using the densities at different temperatures and atmospheric pressure from TRC (1997).

For TEGDME, the parameters of eq 2 were determined by fitting the densities at normal pressure and different temperatures of Esteve et al. (1995b), Svejda et al. (1990), Treszczanowicz et al. (1988), and Tovar (1996). The parameters of eqs 3 and 4 were determined by Cibulka et al.
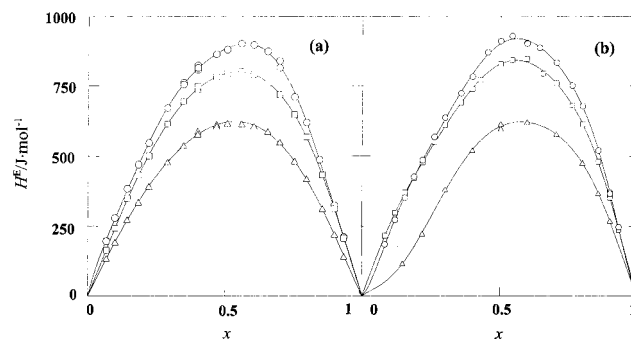

Figure 1. Excess molar enthalpies of the systems (a) x methanol + $(1 - x)$ TEGDME and (b) x methanol + $(1 - x)$ PEGDME 250, at 8 MPa and (○) 423.15 K; (□) 373.15 K; (△) 323.15 K.

(1997) using the isothermal densities at different pressures of Svejda et al. (1990).

The liquid densities of PEGDME 250 were recently determined by some of us (Comunas et al.,1998) using an Anton Paar 502P densimeter, from 283.15 to 323.15 K and up to 10 MPa. The experimental data have also been correlated with eq 1.

Results

The excess molar enthalpies of the binary mixtures of methanol + TEGDME and methanol + PEGDME 250 are listed respectively in Tables 1 and 2. For each binary mixture, a Redlich−Kister polynominal has been used to correlate the experimental values:

$$H^E/\text{J·mol}^{-1} = [x(1 - x)]\sum_i A_i(2x - 1)^i \quad (5)$$

where x is the mole fraction of methanol. The parameters A_i, obtained by a linear least-squares fitting method, are given in Table 3 together with the standard deviations s. The number of coefficients was determined in each case using an F-test. For all the mixtures $s(H^E)/H^E(\text{max}) < 0.01$, where $H^E(\text{max})$ denotes the maximum value of H^E with respect to x. Figure 1 gives the experimental results together with the Redlich−Kister fitted curves.

For both systems, the excess enthalpies are positive over the whole range of composition. The $H^E(x)$ curves are

Table 2. Experimental Excess Molar Enthalpies H^E for the Systems Methanol + PEGDME 250 at 8 MPa and at 323.15 K, 373.15 K, and 423.15 K

x	$H^E/\text{J·mol}^{-1}$	x	$H^E/\text{J·mol}^{-1}$	x	$H^E/\text{·mol}^{-1}$	x	$H^E/\text{J·mol}^{-1}$
			$T = 323.15$ K				
0.1464	115.8	0.3981	515.4	0.5951	612.3	0.8559	363.3
0.2180	221.8	0.4999	591.7	0.7016	571.3	0.8987	267.7
0.2992	378.4	0.5002	604.7	0.7972	470.5		
			$T = 373.15$ K				
0.0829	214.6	0.2605	547.3	0.5000	823.4	0.7590	674.5
0.1202	296.2	0.2994	603.6	0.5415	836.5	0.7972	608.6
0.1549	367.4	0.3572	684.8	0.5950	840.7	0.8558	476.8
0.1875	419.8	0.3983	732.2	0.6537	788.1	0.8987	349.0
0.2181	474.4	0.4264	765.6	0.7016	754.8	0.9315	236.6
			$T = 423.15$ K				
0.0829	184.7	0.2994	630.3	0.5949	8998.0	0.7972	672.3
0.1202	271.1	0.3573	716.7	0.5950	895.8	0.8558	516.3
0.1550	349.5	0.3984	775.6	0.6400	882.7	0.8987	364.1
0.1875	423.8	0.4526	864.9	0.7016	828.0	0.8987	368.3
0.2181	482.0	0.4999	905.4	0.7590	745.7	0.9314	245.8
0.2606	563.2	0.5415	922.7				

Table 3. Parameters A_i for the Redlich−Kister (Eq 5) and Standard Deviations s

	methanol + TEGDME			methanol + PEGDME 250		
	$T/\text{K} = 323.15$	$T/\text{K} = 373.15$	$T/\text{K} = 423.15$	$T/\text{K} = 323.15$	$T/\text{K} = 373.15$	$T/\text{K} = 423.15$
A_0	2473.95	3163.63	3520.75	2394.34	3294.67	3585.88
A_1	381.46	563.51	965.23	850.84	920.00	1202.73
A_2		348.85	994.94	−907.70	−868.26	−1523.30
A_3	−323.98	−164.23	−1088.65	2450.91		
A_4	−460.15	−820.18	−4420.43		3385.48	5559.84
A_5				−2517.08	−701.79	−556.81
A_6			3584.67		−3065.10	−6167.37
s	4.1	3.0	7.2	5.3	4.7	7.5

slightly asymmetrical, and their maximum is skewed to the methanol-rich region. The excess enthalpies increase with increasing temperature. On the contrary, the excess molar volumes V^E of Esteve et al. (1994, 1995b) are negative and decrease as the temperature increases. The pressure dependence of the excess enthalpies can be determined from the excess volumes using the following equation:

$$(\partial H^E/\partial P)_T = V^E - T(\partial V^E/\partial T)_P \quad (6)$$

To determine $(\partial V^E/\partial T)_P$, the experimental V^E values of the methanol + (TEGDME or PEGDME) systems (Esteve et al.,1994, 1995b) at 283.15 K, 293.15 K, 303.15 K, 313.15 K, and 323.15 K were fitted using several equations. Finally, the following equation was chosen to fit the experimental V^E data in both cases (TEGDME and PEGDME 250):

$$V^E/\text{cm}^3\text{·mol}^{-1} = x(1-x)\sum_{i=1}^{4}\sum_{j=1}^{3}B_{ij}10^{j-j}(x/(x+k(1-x)))^{i-1}(T-283.15)^{j-1} \quad (7)$$

Table 4 lists the parameters k and B_{ij} together with the standard deviations. In Figure 2 it can be seen that the fitting curves correlate well the experimental V^E values obtained by Esteve et al. (1994, 1995b).

Figure 3 shows the quantities $(\partial H^E/\partial P)_T$ obtained using the parameters of Table 4 and of eqs 6 and 7. As V^E and $T(\partial V^E/\partial T)_P$ are both negative and of similar magnitude, $(\partial H^E/\partial P)_T$ is small (see eq 6). This implies that a little change in the V^E fitting equation can cause a relatively strong variation on $(\partial H^E/\partial P)_T$. From all the fitting equations that we have used, we conclude that the excess enthalpies

Table 4. Coefficients B_{ij} and k of eq 7 and Standard Deviations s

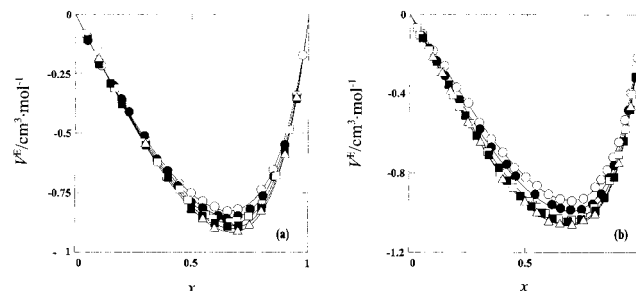|	methanol + TEGDME		
k	4.588227		
B_{ij}	$j = 1$	$j = 2$	$j = 3$
$i = 1$	−1.99287	−5.45099	0.052626
$i = 2$	−0.009323	−0.38494	−0.22867
$i = 3$	0.001472	0.00477	0.06958
s	0.0075		
	methanol + PEGDME 250		
k	2.04099		
B_{ij}	$j = 1$	$j = 2$	$j = 3$
$i = 1$	−1.57171	−0.41352	0.06976
$i = 2$	−5.33596	0.62715	−0.24182
$i = 3$	3.75871	−0.52248	0.43671
$i = 4$	−6.26594	−0.69060	−0.18720
s	0.0088		

Figure 2. Excess molar volumes of Esteve et al. (1994; 1995b) of the systems (a) x methanol + $(1 - x)$ TEGDME and (b) x methanol + $(1 - x)$ PEGDME 250, at atmospheric pressure and (○) 283.15 K; (●) 293.15 K; (□) 303.15 K; (■) 313.15 K; (△) 323.15 K. Curves are calculated by means of eq 7 using the coefficients given in Table 4.

for (methanol + TEGDME or PEGDME 250) change slightly with pressure within the investigated temperature range. Furthermore, the sign of $(\partial H^E/\partial P)_T$ depends on both composition and temperature.
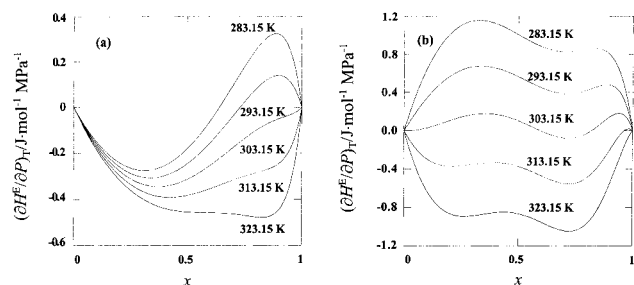
Figure 3. Values of $(\partial H^E/\partial P)_T$ for the systems (a) x methanol $+ (1 - x)$ TEGDME, (b) x methanol $+ (1 - x)$ PEGDME 250 at atmospheric pressure, determined from the experimental excess volumes of Esteve et al. (1994; 1995c) using the equation $(\partial H^E/\partial P)_T = V^E - T(\partial V^E/\partial T)$.

Table 5. Experimental and Calculated H^E at $x = 0.5$ Using Different Models for the System x CH$_3$OH $+ (1 - x)$ TEGDME, at Different Temperatures

			UNIFAC		
T/K	P^a/MPa	exp	(Dortmund)	DISQUAC	Nitta−Chao
298.15	0.1	584	471	791	1330
323.15	8	619	615	973	1881
373.15	8	791	955	1723	2612
423.15	8	880	1377	3279	2874

^{a} The two different pressures indicated are those at which experimental H^E values are available.
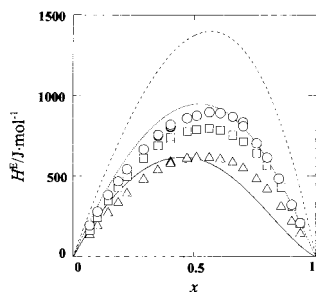

Figure 4. Excess molar enthalpies of x CH$_3$OH $+ (1 - x)$ TEGDME, at 8 MPa and (○) 423.15 K; (□) 373.15 K; (△) 323.15 K. Curves represent the calculated values, at atmospheric pressure, obtained with the UNIFAC (Dortmund) model: (- - -) 423.15 K; (− − −), 373.15 K; (—) 323.15 K.

Calculations of H^E with Group Contribution Models and Conclusion. The experimental enthalpies of the system methanol + TEGDME were compared with the Nitta-Chao, UNIFAC, and DISQUAC calculations of the excess enthalpies and their dependence on temperature. Since the variation of H^E with pressure is small, we have compared the experimental results with the Dortmund version (Weidlich et al., 1987; Gmehling et al., 1993) of UNIFAC and the DISQUAC model (Kehiaian et al.,1989; Gonzalez et al., 1991; Delcros et al., 1995), which are pressure independent. Furthermore, we have applied the Nitta-Chao model, whose predictions depend on pressure (Nitta et al., 1977; Fernandez et al., 1990; Vijande et al., 1997); in this case, the parameters necessary for the calculations were calculated with experimental data at atmospheric pressure (Fernandez et al., 1990; Vijande et al., 1997). Recently Carballo et al. (1997) have checked this model at high pressures for alkanol + alkane mixtures. Table 5 reports the calculations at equimolecular composition corresponding to the three models.

The UNIFAC (Dortmund) model version gives the best predictions, although the agreement becomes worse when the temperature increases, as can be seen in Figure 4.

Literature Cited

Carballo, E.; Peleteiro, J.; Cerdeiriña, C. A.; Tovar, C.; Legido, J. L. Ability of the Nitta-Chao Model for the Prediction of Pressure and Temperature Dependence of the Volumetric Properties of *n*-Alkane + 1-Alkanol Systems. *Fluid Phase Equilib.* **1997**, *133*, 45−55.

Cibulka, I.; Ziková, M. Liquid Densities at Elevated Pressures of 1-Alkanols from C$_1$ to C$_{10}$: A Critical Evaluation of Experimental Data. *J. Chem. Eng. Data* **1994**, *39*, 876−886.

Cibulka, I.; Hnedkovský, L.; Takagi, T. $P-\rho-T$ Data of Liquids: Summarization and Evaluation. 3. Ethers, Ketones, Aldehydes, Carboxilic Acides, and Esters. *J. Chem. Eng. Data* **1997**, *42*, 2−26.

Comuñas, M. J. P.; López, E. R.; Pires, P. F.; Garcia, J.; Fernández, J. Experimental and Predicted Densities of Polyethylene Glycol Dimethyl Ethers between 283.15 K and 313.15 K and up 10 MPa. *Proceedings of VII Encuentro del Grupo Especializado de Termodinámica de la R.S.E.F. y R.S.E.Q.*, Tarragona, Spain, 5−7 June 1998.

Delcros, S.; Quint, J. R.; Grolier, J.-P. E.; Kehiaian, H. V. DISQUAC Calculation of Thermodynamic Properties of Ether + 1-Alkanol Systems. Comparison with UNIFAC Calculation. *Fluid Phase Equilib.* **1995**, *113*, 1−19.

Esteve, X. Transformación de Calor con Sistemas Binarios Metanol + Polietilenglicol Dimetiléter. Ph.D. Thesis, University Rovira i Virgili, Tarragona, Spain, 1995.

Esteve, X.; Boer, D.; Patil, R.; Chaudhari, S. K.; Coronas, A. Densities, Viscosities and Enthalpies of Mixing of the Binary System Methanol + Polyethylene Glycol 250 Dimethyl Ether at 303.15 K. *J. Chem. Eng. Data* **1994**, *39*, 767−769.

Esteve, X.; Chaudhari, S. K.; Coronas, A. Vapor−Liquid Equilibria for Methanol + Tetraethylene Glycol Dimethyl Ether. *J. Chem. Eng. Data* **1995a**, 40, 1252−1256.

Esteve, X.; Olivé, F.; Patil, R.; Chaudhari, S. K.; Coronas, A. Densities and Viscosities of the Binary Mixtures of Interest for Absorption Refrigeration Systems and Heat Pumps. *Fluid Phase Equilib.* **1995b**, *110*, 369−379.

Fernández, J.; Legido, J. L.; Paz-Andrade, M. I.; Pías, L.; Ortega, L. Analysis of Thermodynamic Properties of 1-Alkanol + *n*-Alkane Mixtures Using the Nitta-Chao Contribution Model. *Fluid Phase Equilib.* **1990**, *55*, 293−304.

Gmehling, J.; Li, J.; Schiller, M. A modified UNIFAC model. 2. Present Parameter Matrix and Results for Different Thermodynamic Properties. *Ind. Eng. Chem. Res.* **1993**, *32*, 178−193.

González, J. A.; García de la Fuente, I.; Cobos, J. C.; Casanova, C. A Characterization of the Aliphatic/Hydroxyl Interactions Using a Group Contribution Model (DISQUAC). *Ber. Bunsen-Ges. Phys. Chem.* **1991**, *95*, 1658−1668.

Herraiz, J.; Shen, S.; Coronas, A. Vapor-Liquid Equilibria for Methanol + (Polyethylene Glycol) 250 Dimethyl Ether. *J. Chem. Eng. Data* **1998**, *43*, 191−195.

Kehiaian, H. V.; Tine, M. R.; Lepori, L.; Matteoli, E.; Marongiu, B. Thermodynamics of Binary Mixtures Containing Axaalkanes. Part 3. Monoethers, Polyethers, Acetals, Ortho esters and Cyclic Monoethers + *n*-Alkanes or Cyclohexane. *Fluid Phase Equilib.* **1989**, *46*, 131−177.

Kuczynski, W.; Hart, T.; Westerterp, K. R. Binary Vapour-Liquid Equilibria of Methanol with Sulfolane, Tetraethylene Glycol Dimethyl Ether and 18-Crown-6. *Chem. Eng. Process.* **1986**, *20*, 53−59.

López, E. R.; García, J.; Coronas, A.; Fernández, J. Experimental and Theoretical Excess Enthalpies of the Working Pairs (Methanol or Trifluoroethanol + Polyglycolethers) for Absorption Cycles. *Fluid Phase Equilib.* **1997**, *133*, 229−230.

Mathonat, C.; Hynek, V.; Majer, V.; Grolier, J.-P. E. Measurements of Excess Enthalpies of High Temperature and Pressure Using a New Type of Mixing Unit. *J. Solution Chem.* **1994**, *23*, 1161−1182.

Moncada, L. O.; Giudice, G.; Cotana, F. Latest Developments of Researches on Fluids for Absorption Machines. *Proceedings of CFCs, The Day After*, Padova, Italy, 1994.

Nitta, T.; Turek, E. A.; Greenkorn, E. A.; Chao, K. C. A Group Contribution Molecular Model of Liquids and Solutions. *AIChE J.* **1977**, *23*, 144−150.

Nowaczyk, U.; Steimle, F. Thermophysical Properties of New Working Fluid Systems for Absorption Processes. *Int. J. Refrig.* **1992**, *15*, 10−15.

Svejda, P.; Siddiqi, M. A.; Hahn, G.; Christoph, N. Excess Volume, Isothermal Compressibility, and Excess Enthalpy of the Binary Liquid System 2,2,2,-Trifluoroethanol + 2,5,8,11,14-Pentaoxapentadecane. *J. Chem. Eng. Data* **1990**, *35*, 47−49.

Tovar, C., Estudio Thermodinámico de Mezclas LRquidas de Polioxietilenglicol Dimetil Eteres con Disolventes Orgánicos. Ph.D. Thesis, University of Vigo, Orense, Spain, 1996.

TRC Thermodynamics Tables, Texas A&M University: College Station, Texas, 1997.

Treszczanowicz, T.; Benson, G. C.; Lu, B. C.-Y. Excess Enthalpies for Binary Mixtures 2,5,8-Trioxanonane or 2,5,8,11,14-Pentaoxapentadecane with *n*-Alkanes at 298.15 K. *J. Chem. Eng. Data* **1988**, *33*, 379−381.

Vijande, J.; Legido, J. L.; Iglesias, T. P.; García, J.; Fernández, J. Dependence of the Interaction Parameters with the Molecular Structure Using the Nitta-Chao Model for Ether + 1-Alcohol Mixtures. 15th Experimental Thermodynamics Conference, University of Surrey, Surrey (England), 16−18 April 1997.

Weidlich, U.; Gmehling, J. A Modified UNIFAC Model. 1. Prediction of VLE, h^E, and γ^∞. *Ind. Eng. Chem. Res.* **1987**, *26*, 1372−1381.