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Pair-wise interactions by gas chromatography VI. Interaction free enthalpies of solutes with primary methoxyalkane, cyanoalkane and alkanethiol groups

K.S. Reddy[1], R. Cloux, E. sz. Kováts*

Laboratoire de Chimie Technique, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

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Abstract

Three polar-type liquids, P, having methoxy, cyano or thiol substituents in primary positions on a branched paraffin skeleton were used as stationary phases. The molecules of these stationary liquids have the same form and nearly the same size as that of the non-polar parent branched paraffin, $C_{78}H_{158}$ (C78). Gas chromatographic retention data of some 150 molecular probes were measured on pure P-type liquids and on P/C78 mixtures with a volume fraction φ_P of 0.50. Based on these data interaction free enthalpies could be calculated between a probe and the polar substituent, both at infinite dilution in the alkane solvent.

1. Introduction

The objective of our project is the determination of interaction free enthalpies between molecular probe solutes, *j*, at infinite dilution and an interacting group, X, also at infinite dilution in an alkane solvent. Objective, experimental technique, synthesis of the stationary phases as well as first results have been communicated in Parts I–V of this series [1–5]. The measuring system consists of a family of isosteric, isomorphous solvents, L, shown in Fig. 1. The family includes a standard paraffin, A ≡ C78 ($C_{78}H_{158}$), and a series of polar compounds, P, in which a methyl or an ethyl group is substituted for an interacting group, X. The synthesis of members of this family has been reported in Parts III [3] and IV [4]. The method consists of measuring gas chromatographic data of molecular probes on a series of A–P mixtures at several temperatures, *T*, to convert these data to standard chemical potentials and to extrapolate data to infinite dilution of the interacting group, X [4]. The symbol $\Delta\!\!\!\!-$ will be used throughout the paper to designate additional interaction data, $\Delta\!\!\!\!- Y = \Delta\!\!\!\!- Y^P - \Delta\!\!\!\!- Y^A$, where *Y* is interaction free enthalpy or retention index. The symbol $\Delta\!\!\!\!-'$ will designate data in the hypothetical ideal solvent with reference to data in A ≡ C78, $\Delta\!\!\!\!-'Y = \Delta Y^{idP} - \Delta Y^A \equiv Y^{idP} - Y^A$.

In the present paper we report data on inter-

* Corresponding author.

[1] Present address: Department of Chemistry, S.V. University, Tirupati - 517 502, India.

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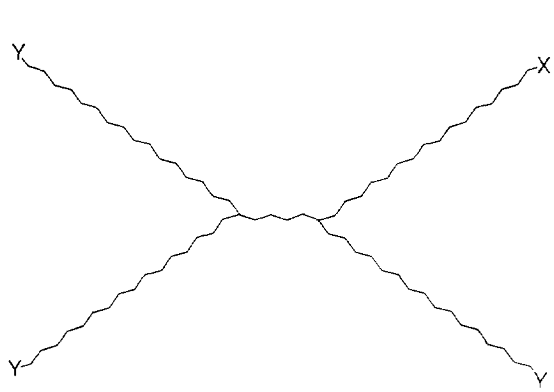

Fig. 1. The structure of the applied stationary phases: C78: $X = Y = CH_2CH_3$; TMO (for tetramethoxy): $X = Y = OCH_3$; PCN (for primary cyano): $X = CH_2CN$, $Y = CH_2CH_3$; PSH (for primary thiol): $X = CH_2SH$, $Y = CH_2CH_3$.

action free enthalpies between molecular probes and methoxy, cyano and thiol moieties as the interacting groups (X). For relationships, theory and symbols as well as for experimental details we refer to Refs. [1] and [4].

2. Experimental

2.1. Materials

For solutes see Ref. [1]. The synthesis of PCN is described in Ref. [3]. For the synthesis of TMO and PSH all the reagents were research-grade compounds from Fluka (Buchs, Switzerland). The stationary liquid TMO was prepared from dimethyl adipate and 16-bromo-1-methoxyhexadecane in an analogous procedure to that described previously [6] and the thiol phase PSH was synthesized from the bromide PBR (preparation see Ref. [3]) and thiourea as described in the following procedures.

11-Bromo-1-methoxyundecane

In a 250-ml 2-necked round-bottom flask equipped with a dropping funnel and a reflux condenser Mg (7.5 g, 0.31 mol) was covered with tetrahydrofuran (THF) (30 ml), activated with 1,2-dibromoethane (0.94 g, 5.0 mmol) and a solution of 1-bromobutane (27.4 g, 200 mmol) in THF (50 ml) was added dropwise.[1] At the end of the introduction THF (100 ml) was added and the reaction mixture was refluxed for 2.0 h. In a second 500-ml 2-necked round-bottom flask equipped with a reflux condenser and a dropping funnel 11-bromo-1-undecanol (50.2 g, 200 mmol) was dissolved in THF (100 ml) and dimethyl sulfate (50.4 g, 400 mmol) was added. The Grignard reagent from the first flask was now transferred into the dropping funnel and added within 20 min to the bromoalcohol. The mixture was refluxed for 28 h, cooled to room temperature and the excess dimethylsulfate was hydrolyzed with half-saturated aqueous $KHCO_3$ (200 ml). The organic layer was washed with brine (100 ml), the aqueous phase was extracted with diethyl ether (2×100 ml) and the combined organic phase was dried (Na_2SO_4). The solvent was distilled in a rotary evaporator to give 57.1 g of crude 11-bromo-1-methoxyundecane which was dissolved in hexane (100 ml) and filtered on silica gel (100 g) with hexane–diethyl ether (9:1, 600 ml) as mobile phase to afford 51.1 g of colorless liquid. Distillation at 82.5–83.5°C/ 1.8×10^{-2} mbar gave 46.3 g (87%) of pure 11-bromo-1-methoxyundecane. (GC: 98.9% pure, $I_{200} = 1695$). IR (film): $\nu/cm^{-1} = 2920$, 2850, 1465, 1385, 1120, 725, 645 and 570. ^1H NMR (C^2HCl_3, TMS): $\delta/ppm = 1.28$ (m, 14 protons ≡ H), 1.58 (m, 2H), 1.85 (quint., 2H, $J = 7.1$ Hz), 3.33 (s, 3H), 3.36 (t, 2H, $J = 6.5$) and 3.41 (t, 2H, $J = 6.9$). ^{13}C NMR (C^2HCl_3, TMS): $\delta/ppm = 26.12$, 28.16, 28.73, 29.38, 29.44, 29.50, 29.63, 32.85, 33.80, 58.44 and 72.94. MS (EI): $m/z = 266$ ($M^+ + 2$, 0.1% of 45), 264 (M^+, 0.1), 234 (4), 232 (4), 164 (9), 162 (9), 150 (11), 148 (11), 97 (20), 83 (35), 69 (38), 55 (38) and 45 (100).

16-Bromo-1-methoxyhexadecane

In a 500-ml 2-necked round-bottom flask Mg (4.86 g, 200 mmol) was covered with THF (150 ml) and activated with 1,2-dibromoethane (1.88 g, 10.0 mmol). A solution of 11-bromo-1-

[1] In this reaction the Grignard reagent of 1-bromobutane has been used as a base instead of KOH or the like. Hydroxyl bases would produce 1,11-undecanediol and oxacyclododecane as side products.

methoxyundecane (26.5 g, 100 mmol) in THF (100 ml) was added dropwise in 15 min and the mixture was refluxed for 1.5 h. In a second 1-l 2-necked round-bottom flask equipped with a dropping funnel and an Ar line 1,5-dibromopentane (69.0 g, 300 mmol) was dissolved in THF (250 ml). Li_2CuCl_4 (1 *M*) in THF (1.0 ml, 1.0 mmol; Kochi's reagent [7]) was added and the bright yellow solution was cooled to 0°C (ice bath). The Grignard reagent from the first flask was transferred into the dropping funnel and added slowly to the cold reaction mixture over a 1.0-h period. The mixture was stirred for 3.0 h at 0°C then it was allowed to warm to room temperature where it was stirred for another 2.0 h. Then it was hydrolyzed with saturated aqueous NH_4Cl (200 ml). The organic phase was washed with a second portion of saturated aqueous NH_4Cl (200 ml) then with brine (200 ml). The aqueous layer was extracted with diethyl ether (200 ml) and the combined organic phase was dried (Na_2SO_4). The solvent was removed in a rotary evaporator and the residue was chromatographed on silica gel (300 g). Hexane (2.0 l) eluted the excess 1,5-dibromopentane. The desired 16-bromo-1-methoxyhexadecane was eluted with a mixture of hexane–diethyl ether (90:10, 600 ml). Recrystallization from 94 wt% ethanol at 0°C gave 22.2 g (66%) of pure 16-bromo-1-methoxyhexadecane as colorless plates with a m.p. of 27.5–28.5°C. (GC: 99.4% pure, $I_{220} = 2204$). IR (CCl_4, CS_2): ν/cm^{-1} = 2930, 2850, 1465, 1385, 1120, 720, 645 and 570. ^1H NMR (C^2HCl_3, TMS): δ/ppm = 1.27 (m, 24 protons ≡ H), 1.54 (m, 2H), 1.85 (quint., 2H, J = 7.2 Hz), 3.34 (s, 3H), 3.37 (t, 2H, J = 6.6) and 3.42 (t, 2H, J = 6.9). ^{13}C NMR (C^2HCl_3, TMS): δ/ppm = 26.15, 28.19, 28.77, 29.42, 29.50, 29.52, 29.59, 29.63, 32.88, 33.83, 58.46 and 72.98. MS (EI): m/z = 337 (M^+ + 3, 0.1% of 45), 336 (M^+ + 2, 0.1), 335 (M^+ + 1, 0.1), 334 (M^+, 0.1), 304 (7), 302 (7), 150 (11), 148 (11), 97 (49), 83 (65), 69 (63), 55 (72), 45 (100).

17,22-Bis-(16-methoxyhexadecyl)-1,38-dimethoxy-17,22-octatriacontanediol (TMO-diol)

In a 250-ml 2-necked round-bottom flask equipped with a magnetic stirrer, a dropping funnel and a reflux condenser Mg (3.2 g, 132 mmol) was covered with THF (70 ml) and activated with 1,2-dibromoethane (0.94 g, 5.0 mmol). A solution of 16-bromo-1-methoxyhexadecane (22.13 g, 66.0 mmol) in THF (50 ml) was added dropwise within 30 min and the reaction mixture was refluxed for 2.0 h. At the same temperature a solution of dimethyladipate (2.61 g, 15.0 mmol) in THF (10 ml) was added dropwise and the reflux was maintained for 5.0 h. The reaction mixture was cooled to room temperature and hydrolyzed with half-saturated aqueous NH_4Cl (100 ml). The organic phase was washed with brine (100 ml) and the aqueous phases were extracted with hexane (100 ml). The combined organic phase was dried (Na_2SO_4) and the solvent was distilled in a rotary evaporator to give 18.6 g of crude TMO-diol. The latter was dissolved in hexane (100 ml) and chromatographed on silica gel (100 g). Elution with benzene (1000 ml) afforded 4.54 g of a mixture of 1-methoxyhexadecane and 1,32-dimethoxydotriacontane. Elution with hexane–diethyl ether (1:1, 1000 ml) gave 13.56 g of TMO-diol. Recrystallization from abs. EtOH (400 ml) at 0°C gave 12.2 g (72%) of TMO-diol containing ca. 5% of a ketonic impurity that was removed in the next step; m.p. 63–63.5°C. IR (CCl_4, CS_2): ν/cm^{-1} = 2930, 2850, 1465, 1385, 1195, 1120, 965 and 720. ^1H NMR (C^2HCl_3, TMS): δ/ppm = 1.26 (m, 120 protons ≡ H), 1.57 (quint., 8H, J = 6.4 Hz), 3.34 (s, 12H) and 3.37 (t, 8H, J = 6.5). ^{13}C NMR (C^2HCl_3, TMS): δ/ppm = 23.50, 24.12, 26.14, 29.49, 29.59, 29.65, 30.30, 39.33, 58.43, 72.97 and 74.33.

17,22-Bis-(16-methoxyhexadecyl)-1,38-dimethoxyoctatriacontane (TMO)

In a 250-ml round-bottom flask equipped with a Dean-Stark trap TMO-diol (11.52 g, 10.14 mmol), and *p*-toluenesulfonic acid monohydrate (0.39 g, 2.0 mmol) were dissolved in benzene (100 ml) and the water was removed by heating the solution to reflux for 9.0 h. The reaction mixture was then cooled to room temperature and successively washed with H_2O (50 ml), half-saturated aqueous $KHCO_3$ (50 ml). The aqueous phases were extracted with hexane (100 ml), the combined organic phase was dried (Na_2SO_4) and the solvent was removed in a rotary evaporator. The residue (11.37 g) was dissolved in a mixture of ethanol–cyclohexane (5:1, 120 ml), sodium borohydride (0.37 g, 10.0 mmol) was added and the reaction mixture was heated to 50°C for 30 min. The solvent was then removed in a rotary evaporator, the residue was extracted with cyclohexane (100 ml) and filtered on silica gel (30 g). Elution with benzene (300 ml) followed by cyclohexane–diethyl ether (95:5, 200 ml) afforded 6.84 g of TMO-diene. The latter was dissolved in cyclohexane (400 ml), 10% Pd-C (0.32 g) was added and the reaction mixture was hydrogenated at 40°C under 11 bar H_2 pressure for 18.0 h. The catalyst was removed by filtration on silica gel (30 g). Elution with a mixture of cyclohexane–diethyl ether (50:50, 200 ml) gave after evaporation of the solvent 6.50 g of TMO that was recrystallized from a mixture of ethanol–hexane (8:3, 110 ml) to give 6.21 g (55%) of pure TMO; mp 64.5–67.5°C. IR (CCl_4, CS_2): $\nu/cm^{-1} = 2930$, 2850, 1465, 1385, 1120 and 720. ^1H NMR (C^2HCl_3, TMS): δ/ppm = 1.26 (m, 122 protons ≡ H), 1.58 (m, 8 H), 3.34 (s, 12 H) and 3.37 (t, 8H, $J = 6.5$ Hz). ^{13}C NMR (C^2HCl_3, TMS): δ/ppm = 26.16, 26.77, 27.19, 29.51, 29.61, 29.71, 30.17, 33.80, 37.47, 58.46 and 72.99.

18,23-Dioctadecyl-1-untetracontanylthiouronium bromide (PSTHIU)

In a 250-ml round-bottom flask 1-bromo-18,23-dioctadecyluntetracontane (PBR, 6.60 g, 5.68 mmol) and thiourea (2.16 g, 28.4 mmol) were suspended in a mixture of cyclohexane–ethanol (1:2, 90 ml) and the reaction mixture was heated to reflux for 24 h (the mixture becomes homogeneous after ca. 4 h) and was allowed to cool to room temperature. The solvent was removed in a rotary evaporator and the solid residue was extracted with hot cyclohexane (50–60°C, 3 × 50 ml). The solvent was evaporated and the residue was recrystallized from ethanol–hexane (2:1, 90 ml) to give 6.86 g (98%) of a white solid, m.p. 143.5–144.5°C. ^1H NMR (C^2HCl_3, TMS): δ/ppm = 0.89 (t, 9 protons ≡ H, $J = 6.4$ Hz), 1.25 (m, 142 H), 1.74 (quint., 2 H, $J = 7.2$), 3.32 (t, 2 H, $J = 7.2$). ^{13}C NMR (C^2HCl_3, TMS): δ/ppm = 14.05, 22.67, 26.77, 26.83, 27.21, 28.24, 28.46, 29.05, 29.35, 29.41, 29.71, 30.17, 31.93, 32.31, 33.82, 37.50 and 172.57.

18,23-Dioctadecyl-1-untetracontanethiol (PSH)

In a 250-ml round-bottom flask equipped with a reflux condenser PSTHIU (6.78 g, 5.48 mmol) was dissolved in ethanol–cyclohexane (2:1, 75 ml) and a solution of KOH (0.72 g, 11 mmol) in H_2O (4 ml) was added. The reaction mixture was heated to reflux for 1.0 h then stirred at room temperature overnight. The mixture was diluted with cyclohexane (100 ml), washed with H_2O (3 × 50 ml) and the organic phase was dried (Na_2SO_4). The solvent was distilled in a rotary evaporator and the residue was chromato-

Table 1
Physical properties of the stationary phases

L		m.p. (°C)	M ($g\,mol^{-1}$)	$\rho^{\dagger}$ ($g\,cm^{-3}$)	$v^{\dagger}$ ($cm^3\,mol^{-1}$)	$\alpha^{\dagger} \cdot 10^4$ (K^{-1})	$B \cdot 10^7$ (K^{-2})	σ ($g\,cm^{-3}$)
Symbol	Formula							
C78	$C_{78}H_{158}$	69–75	1096.1	0.7714	1420.9	7.62	1.26	0.0004
TMO	$C_{70}H_{138}(OCH_3)_4$	65–68	1104.0	0.8039	1373.3	7.82	2.51	0.0004
PCN	$C_{77}H_{155}CN$	66–68	1107.1	0.7826	1414.7	7.64	1.64	0.0003
PSh	$C_{77}H_{155}SH$	70–74	1114.2	0.7870	1415.7	7.64	1.31	0.0002
Δ_{95}				±0.00009	±0.17	±0.34	±0.93	

The symbol m.p. is for melting point and M is for molar mass; the symbols $p^{\dagger}$, $\alpha^{\dagger}$ and B are regression coefficients of Eq. (1) for the calculation of the density in the temperature domain 80–210°C; $v^{\dagger}$ is for the molar volume at the standard temperature $T^{\dagger} = 403.15$K. Data for C78 are from Ref. [8], those for PCN are from Ref. [3].

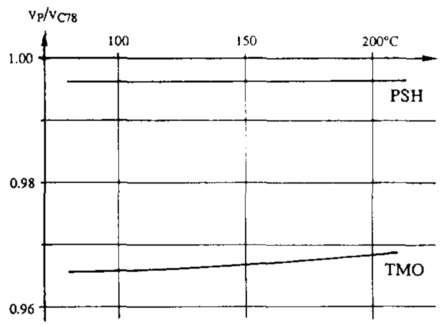

Fig. 2. Ratio of the molar volume of the P and C78 stationary phases as a function of temperature. P: TMO and PSH.

graphed on silica gel (100 g) with cyclohexane as mobile phase. Bis-(18,23-dioctadecyl-1-untetracontanyl)sulfide (1.2 g) was obtained as a first fraction followed by PSH (4.05 g). Recrystallization from ethanol–cyclohexane (2:1, 60 ml) at 0°C afforded 3.98 g (65%) of pure thiol as a white powder, m.p. 70.5–73.5°C. ^{1}H NMR (C^2HCl_3, TMS): δ/ppm = 0.89 (t, 9 protons ≡ H, J = 6.4 Hz), 1.27 (m, 142 H), 1.82 (quint. 2 H, J = 7.4) and 2.53 (q, 2H, J = 7.3). ^{13}C NMR (C^2HCl_3, TMS): δ/ppm = 14.06, 22.68, 24.62, 26.79, 26.95, 27.22, 28.41, 29.10, 29.36, 29.55, 29.73, 30.19, 31.94, 33.84, 34.08 and 37.51.

Table 2
Characteristics of the chromatographic columns

A/P	$100\varphi_P^\dagger$ (%)	w_L (g)	P_L (%)
C78/TMO	50.0 (a)	1.798	6.48
	50.0 (b)	0.959	5.89
	100 (a)	1.787	6.44
	100 (b)	0.980	5.96
C78/PCN	50.0	1.750	6.26
	100	1.665	6.23
C78/PSH	50.0	1.761	5.28
	100	1.864	5.52

The symbol $\varphi_P^\dagger$ is for the volume fraction of the polar solvent in the A/P mixture at 130°C; w_L is for the mass of the stationary liquid in the column and P_L is for the weight percent of L of the packing ($100w_L$/total mass).

Densities

Densities were measured as described in part IV [4] in the temperature range of 80–200°C. Eq. (1) was fitted to the experimental points

$$\ln \rho_L = \ln M_L - \ln v_L = \ln \rho^\dagger - \alpha^\dagger \Delta T - B\,\Delta T^2 \tag{1}$$

where $\rho^\dagger$ is the density and $\alpha^\dagger$ is the isobaric coefficient of thermal expansion at $T^\dagger = 130.0 + 273.15 = 403.15$ K. Coefficients of Eq. (1) for the stationary liquids are listed in Table 1. Fig. 2 shows that the ratio of the molar volumes of the stationary phases TMO and PSH is reasonably near unity. Characteristics of the columns used in this work are summarized in Table 2.

2.2. Apparatus

See part I [1] and IV [4].

2.3. Retention data

Alkanes

As in Refs. [1] and [4] absolute retention data of n-alkanes, C_zH_{2z+2}, with $5 \leq z \leq 10$ were determined in the temperature range 90–210°C. Specific retention volumes on the stationary phases C78/TMO and TMO were determined on two columns (a and b in Table 2). Data were converted to chemical potentials and those on

Table 3
Average ratio of specific retention volumes on columns of series (a) and (b): $f = V_g^{(b)}/V_g^{(a)}$, and the corresponding corrections to add to standard chemical potentials determined on columns of series (a)

L	f	$0.5RT \ln f$(cal mol^{-1})						
		90	110	130	150	170	190	210°C
C78/TMO	0.989	−4.0	−4.2	−4.4	−4.7	−4.9	−5.1	−5.3
TMO	1.004	+1.4	+1.5	+1.6	+1.7	+1.8	+1.8	+1.9

TMO were corrected to the average of the two columns following the method given in Ref. [4]; corrections are given in Table 3. Variance analyses of the resulting data sets are shown in Tables 4, 5 and 6. Based on the variance analysis n-alkane data were fitted to the following equation:

$$\Delta\mu_z^{A/P} = \Delta\mu_0^{\dagger,A} + z\,\delta\mu_z^{\dagger,A} - \Delta T\,\Delta S_0^A - \Delta Tz\,\delta S_z^A - \Delta T^2 \frac{\Delta C_{P,0}^A}{2T^\dagger} - \Delta T^2 z \frac{\delta C_{P,z}^A}{2T^\dagger} + \varphi_P\,\Delta\mu_0^{\dagger,P} + \varphi_P z(\delta\mu_z^{\dagger,P} - \delta\mu_z^{\dagger,A}) - \Delta T\varphi_P \Delta S_0^P - \Delta T\varphi_P z(\delta S_z^P - \delta S_z^A)$$

Table 4
Analysis of variance of the set of 126 standard chemical potentials of the n-alkane solutes with $5 \leq z \leq 10$ in the temperature range 90–210°C at three compositions of the C78/TMO mixture

Source		SQ	Φ	V'	F	Sign. (%)	$b_X^{(i)}$	Function
X	(i)							
$\Delta\bar{\mu}$	(0)						42.5	$\Delta\mu_0^{\dagger,A}$
T	(1)	2 195.8	1	id	$6.55 \cdot 10^1$	0.1	2.09	ΔS_0^A
	(2)	260.2	1	id	7.77	5	− 0.411	$\Delta C_{P,0}^A$
	(res. T*	261.0	4	65.3	1.95	20)		
L	(1)	116 935.5	1	id	$3.49 \cdot 10^3$	0.01	37.310	$\Delta\mu_0^{\dagger,P}$
	(2)	6 783.9	1	id	$2.03 \cdot 10^2$	0.1	−15.569	$m_0^{\dagger,A/P}$
TL	(1, 1)	542.9	1	id	$1.62 \cdot 10^1$	1	1.268	ΔS_0^P
	(1, 2)	671.5	1	id	$2.00 \cdot 10^1$	0.1	− 2.451	$s_0^{A/P}$
	(2, 1)	121.3	1	id	3.62	10	− 0.490	$\Delta C_{P,0}^P$
	(res. TL*	174.5	9	19.4	0.58	–)		
1st res.	(=Σ X*)	435.5	13	33.5				
Z	(1)	2 892.1	1	id	$2.75 \cdot 10^2$	0.01	2.8	$\delta\mu_z^{\dagger,A}$
	(2)	537.8	1	id	$5.12 \cdot 10^1$	0.1	− 0.832	
	(3)	207.4	1	id	$1.97 \cdot 10^1$	0.1	0.391	
	(res. Z**	35.6	2	17.8	1.69	20)		
TZ	(1, 1)	181.5	1	id	$1.73 \cdot 10^1$	0.1	0.352	δS_z^A
	(2, 1)	28.7	1	id	2.73	20	− 0.083	$\delta C_{P,z}^A$
	(res. TZ**	291.9	28	10.4	0.99	–)		
LZ	(1, 1)	1 244.4	1	id	$1.19 \cdot 10^2$	0.1	2.252	$\delta\mu_z^{\dagger,P}$
	(2, 1)	223.7	1	id	$2.13 \cdot 10^1$	0.1	− 1.650	$\delta m_z^{\dagger,A/P}$
	(res. LZ**	408.7	8	51.1	4.87	5)		
TLZ	(1, 1, 1)	49.9	1	id	4.75	5	0.232	δS_z^P
	(2, 1, 1)	5.8	1	id	0.55	–	− 0.041	$\delta C_{P,z}^P$
	(1, 2, 1)	79.0	1	id	7.52	1	− 0.489	$\delta s_z^{A/P}$
	(res. TLZ**	258.8	57	4.5	0.43	–)		
2nd res.	(=Σ X**)	995.0	95	10.5				

* Sum of the residuals marked by one asterisk.
** Sum of the residuals marked by two asterisks.
$X^{(i)}$ is the systematic polynomial variation of $\Delta\mu^{A/P}$ on the effects T (temperature), L (composition of the liquid stationary phase, $100\,\varphi_P$ = 0.0, 50.0 and 100.0%) and Z (carbon number of the solute). The subscripts in parentheses refer to the degree of the orthogonal polynomial: (1) linear; (2) quadratic; (3) cubic. SQ is the sum of squares, Φ is the number of degrees of freedom and $V' = V\text{(res.)} + \nu_X V(X)$ is the combined variance to be analysed by Fisher's F (ν_X is the number of statistical units in one datum of the subset used for the evaluation of the effect) [9]. The values of the coefficients $b_X^{(i)}$ are also listed along with the corresponding thermodynamic coefficients. The meaning of the symbols of thermodynamic functions are described in the text. The abbreviations "res." is for residual variance, "sign." is for significance level and "id." means that $V' = SQ/\Phi$ is equal to the corresponding SQ ($\Phi = 1$).

Table 5
Analysis of variance of the set of 126 standard chemical potentials of the n-alkane solutes with $5 \leq z \leq 10$ in the temperature range 90–210°C at three compositions of the C78/PCN mixture

Source X	(i)	SQ	Φ	V'	F	Sign. (%)	$b_X^{(i)}$	Function
$\Delta\bar{\mu}$	(0)						66.8	$\Delta\mu_0^{\dagger,A}$
T	(1)	3 051.3	1	id	$1.01 \cdot 10^2$	0.1	2.46	ΔS_0^A
	(2)	131.9	1	id	4.35	10	0.295	$\Delta C_{P,0}^A$
	(res. T*	12.3	4	3.1	0.10	–)		
L	(1)	306 167.7	1	id	$1.01 \cdot 10^4$	0.01	60.373	$\Delta\mu_0^{\dagger,P}$
	(2)	10 300.2	1	id	$3.39 \cdot 10^2$	0.1	−19.179	$m_0^{\dagger,A/P}$
TL	(1, 1)	443.7	1	id	$1.46 \cdot 10^1$	1	1.151	ΔS_0^P
	(1, 2)	1 733.6	1	id	$5.72 \cdot 10^1$	0.1	− 3.930	$s_0^{A/P}$
	(2, 1)	63.1	1	id	2.08	20	0.252	$\Delta C_{P,0}^P$
	(res. TL*	381.9	9	42.4	1.40	–)		
1st res.	(=Σ X*)	394.2	13	30.3				
Z	(1)	3 011.2	1	id	$2.03 \cdot 10^2$	0.1	2.9	$\delta\mu_z^{\dagger,A}$
	(2)	1 614.7	1	id	$1.09 \cdot 10^2$	0.1	− 1.435	
	(3)	581.7	1	id	$3.93 \cdot 10^1$	0.1	0.654	
	(res. Z**	119.0	2	59.5	4.02	10)		
TZ	(1, 1)	227.6	1	id	$1.54 \cdot 10^1$	0.1	0.391	δS_z^A
	(2, 1)	163.6	1	id	$1.11 \cdot 10^1$	1	− 0.189	$\delta C_{P,z}^A$
	(res. TZ**	44.4	28	1.6	0.11	–)		
LZ	(1, 1)	1 570.8	1	id	$1.06 \cdot 10^2$	0.1	2.531	$\delta\mu_z^{\dagger,P}$
	(2, 1)	80.2	1	id	5.42	5	− 0.990	$\delta m_z^{\dagger,A/P}$
	(res. LZ**	1 158.7	8	144.8	9.78	1)		
TLZ	(1, 1, 1)	65.3	1	id	4.41	5	0.261	δS_z^P
	(2, 1, 1)	30.4	1	id	2.05	20	− 0.102	$\delta C_{P,z}^P$
	(1, 2, 1)	53.8	1	id	3.64	10	− 0.411	$\delta s_z^{A/P}$
	(res. TLZ**	84.6	57	1.5	0.10	–)		
2nd res.	(=Σ X**)	1 406.7	95	14.8				

* Sum of the residuals marked by one asterisk.
** Sum of the residuals marked by two asterisks.
For explanation of symbols see Table 4.

$$- \Delta T^2 \varphi_P \frac{\Delta C_{P,0}^P}{2T^\dagger} - \Delta T^2 \varphi_P z \frac{\delta C_{P,z}^P - \delta C_{P,z}^A}{2T^\dagger}$$
$$+ \varphi_A \varphi_P m_0^{\dagger,A/P} + \varphi_A \varphi_P z \, \delta m_z^{\dagger,A/P}$$
$$- \Delta T \varphi_A \varphi_P s_0^{A/P} - \Delta T \varphi_A \varphi_P z \, \delta s_z^{A/P} \qquad (2)$$

Numerical values of the coefficients in Eq. (2) are listed in Table 7. The value of the derivative of Eq. (2) at zero concentration of the polar partner, P, gives the standard chemical potential of n-alkanes at ideal dilute solution of the functional group (see Ref. [1]) to give

$$\Delta'\mu_z^{idP} = \Delta'\mu_0^{\dagger,idP} + z\,\delta'\mu_z^{\dagger,idP} - \Delta T\,\Delta' S_0^{idP}$$
$$- \Delta T z\,\delta' S_z^{idP} - \Delta T^2 \frac{\Delta' C_{P,0}^{idP}}{2T^\dagger}$$
$$- \Delta T^2 z \frac{\delta' C_{P,z}^{idP}}{2T^\dagger} \qquad (3)$$

Numerical values of the coefficients in Eq. (3) are listed in Table 7. The derivative of Eq. (2) with respect of the carbon number, z, gives the necessary equations for the "methylene increment" as follows

Table 6
Analysis of variance of the set of 126 standard chemical potentials of the n-alkane solutes with $5 \leq z \leq 10$ in the temperature range 90–210°C at three compositions of the C78/PSH mixture

Source		SQ	Φ	V'	F	Sign. (%)	$b_X^{(i)}$	Function
X	(i)							
$\Delta\bar{\mu}$	(0)						60.8	$\Delta\mu_0^{\dagger,A}$
T	(1)	161.4	1	id	1.41	–	0.57	ΔS_0^A
	(2)	108.1	1	id	0.95	–	0.267	$\Delta C_{P,0}^A$
	(res. T*	636.5	4	159.1	1.39	–)		
L	(1)	243 822.1	1	id	$2.13 \cdot 10^3$	0.01	53.876	$\Delta\mu_0^{\dagger,P}$
	(2)	12 088.9	1	id	$1.06 \cdot 10^2$	0.1	−20.779	$m_0^{\dagger,A/P}$
TL	(1, 1)	183.6	1	id	1.61	–	0.739	ΔS_0^P
	(1, 2)	30.3	1	id	0.27	–	0.520	$s_0^{A/P}$
	(2, 1)	114.6	1	id	1.00	–	0.337	$\Delta C_{P,0}^P$
	(res. TL*	848.9	9	94.3	0.82	–)		
1st res.	(=Σ X*)	1 485.4	13	114.3				
Z	(1)	11 805.9	1	id	$8.08 \cdot 10^2$	0.01	5.7	$\delta\mu_z^{\dagger,A}$
	(2)	1 399.8	1	id	$9.59 \cdot 10^1$	0.1	− 1.336	
	(3)	485.3	1	id	$3.32 \cdot 10^1$	0.1	0.597	
	(res. Z**	97.9	2	48.9	3.35	5)		
TZ	(1, 1)	224.5	1	id	$1.54 \cdot 10^1$	0.1	0.391	δS_z^A
	(2, 1)	0.0	1	id	0.00	–	0.000	$\delta C_{P,z}^A$
	(res. TZ**	131.7	28	4.7	0.32	–)		
LZ	(1, 1)	4 249.0	1	id	$2.91 \cdot 10^2$	0.1	4.164	$\delta\mu_z^{\dagger,P}$
	(2, 1)	1 661.3	1	id	$1.14 \cdot 10^2$	0.1	− 4.510	$\delta m_z^{\dagger,A/P}$
	(res. LZ**	1 027.4	8	128.4	8.79	0.1)		
TLZ	(1, 1, 1)	75.9	1	id	5.19	1	0.278	δS_z^P
	(2, 1, 1)	24.5	1	id	1.68	20	0.091	$\delta C_{P,z}^P$
	(1, 2, 1)	37.1	1	id	2.54	10	− 0.337	$\delta s_z^{A/P}$
	(res. TLZ**	127.8	57	2.2	0.15	–)		
2nd res.	(=Σ X**)	1 384.8	95	14.6				

* Sum of the residuals marked by one asterisk.
** Sum of the residuals marked by two asterisks.
For explanation of symbols see Table 4.

$$\delta\mu_z^A = -510.5 + 1.2379\,\Delta T - 0.00244\,\Delta T^2 \quad (4a)$$

$$\delta\mu_z^{TMO} = -506.0 + 1.2745\,\Delta T - 0.00262\,\Delta T^2 \quad (4b)$$

$$\delta\mu_z^{PCN} = -507.4 + 1.2784\,\Delta T - 0.00263\,\Delta T^2 \quad (4c)$$

$$\delta\mu_z^{PSH} = -504.4 + 1.2288\,\Delta T - 0.00209\,\Delta T^2 \quad (4d)$$

"Methylene increments" for ideal polar solvents derived from Eq. (3) are as follows

$$\delta'\mu_z^{idMeO} = -506.8 + 1.2533\,\Delta T - 0.00249\,\Delta T^2 \quad (5a)$$

$$\delta'\mu_z^{idPCN} = -504.3 + 1.2998\,\Delta T - 0.00267\,\Delta T^2 \quad (5b)$$

$$\delta'\mu_z^{idPSH} = -481.0 + 1.2477\,\Delta T - 0.00195\,\Delta T^2 \quad (5c)$$

Let us note that the variance analyses refer to the approximate expression given in Eq. (2) which is the Taylor series of Eq. (6), where

Table 7
Coefficients for the description of the chemical potential of n-alkanes in real A/P mixtures, Eq. (2), and in ideal solution of the primary polar substituents, Eq. (3)

Eq. (2)				Eq. (3)			
P:	TMO	PCN	PSH	idP;	MeO	PCN	PSH
$\Delta\mu_0^{\dagger,A}$	3465.8	3465.8	3465.8	$\Delta'\mu_0^{\dagger,idP}$	3481.1	3672.2	3511.5
$\delta\mu_z^{\dagger,A}$	−510.49	−510.49	−510.49	$\delta'\mu_z^{\dagger,idP}$	−506.78	−504.30	−481.03
ΔS_0^A	−9.712	−9.712	−9.712	$\Delta' S_0^{idP}$	−9.865	− 10.461	−9.733
δS_z^A	−1.2379	−1.2379	−1.2379	$\delta' S_z^{idP}$	−1.2533	−1.2998	−1.2477
$\Delta C_{P,0}^A$	−3.47	−3.47	−3.47	$\Delta' C_{P,0}^{idP}$	−3.47	−9.51	−0.65
$\delta C_{P,z}^A$	1.967	1.967	1.967	$\delta' C_{P,z}^{idP}$	2.008	2.153	1.572
$\Delta\mu_0^{\dagger,P}$	43.3	93.9	57.4				
$\delta\mu_z^{\dagger,P} - \delta\mu_z^{\dagger,A}$	4.09	3.08	6.12				
ΔS_0^P	0.080	0.214	−0.067				
$\delta S_z^P - \delta S_z^A$	−0.0366	−0.0405	0.0091				
$\Delta C_{P,0}^P$	0.40	−3.95	2.02				
$\delta C_{P,z}^P - \delta C_{P,z}^A$	0.145	0.153	−0.282				
$m_0^{\dagger,A/P}$	2.2	52.4	− 25.9				
$\delta m_z^{\dagger,A/P}$	6.63	1.26	14.73				
$s_0^{A/P}$	−0.489	−0.627	0.073				
$\delta s_z^{A/P}$	0.0	0.0	0.0				

Kirchhoff's approximation is used for the temperature dependence of ΔH and ΔS.

$$\Delta\mu_j^{A/P} = \varphi_P\left[\Delta H_j^P - T\Delta S_j^P + \Delta C_{P,j}^P \times \left(T - T^{\dagger} - T\ln\frac{T}{T^{\dagger}}\right)\right] + \varphi_A\varphi_P(h_j - Ts_j) \quad (6)$$

In Tables 8, 9 and 10 results are listed. Data given under the heading "Thermodynamic data" refer to the coefficients in Eq. (6), which were obtained by non linear multiple regression.

Other solutes

For all *other solutes* retention indices were determined. Data in Tables 8, 9 and 10 describing the dependence of retention indices on composition and temperature are regression coefficients of Eq. (7)

$$\Delta I_j^P = I_j^P - I_j^A = \varphi_P(\Delta I_{130,j} + \Delta A_{T,j}\,\Delta T + \Delta A_{TT,j}\,\Delta T^2) + \varphi_A\varphi_P(A_{L,j} + A_{LT,j}\,\Delta T) \quad (7)$$

Retention indices were reconverted point by point to standard chemical potentials with the aid of n-alkane data (Eqs. 2 and 3) and Eq. (6) was fitted on the resulting data sets. Regression coefficients are listed under the heading "Thermodynamic data" in Tables 8, 9 and 10.

3. Results and discussion

The excess standard chemical potential of a solute in an A/P-mixture with respect to that in pure A ≡ C78 is described by Eq. (8)

$$\Delta\mu_j^{A/P} = \varphi_P\,\Delta\mu_j^P + \varphi_A\varphi_P m_j^{A/P} \quad (8)$$

i.e. this function is (slightly) curved, the extent of curvature being characterized by the constant $m_j^{A/P}$ For the experimental determination of this constant retention of solute j must be determined on at least three A/P-mixtures of different compositions (in our case $\varphi_P = 0$, 1/2 and 1). Knowledge of this constant is necessary to calculate the $\Delta'\mu$-value of a compound which is the difference of the std. chemical potential measured on a hypothetical stationary phase of a one molar ideal solution of the interacting group, X, in C78 and the same parameter on pure C78. Experimental evidence shows that the constant $m_j^{A/P}$ can be correlated with the standard chemi-

Table 8
Retention indices and thermodynamic data for 152 solutes in C78/TMO mixtures where data on an ideal solvent, a one molar solution of X = MeO, idMeO, are also given.
The symbol n is for the number of data points used for regression where points for pure C78 were taken from Refs. [1,4,5]. Constants and functions, Y, preceded by Δ refer to those on C78, i.e. $\Delta Y(\mathrm{P}) = Y(\mathrm{P}) - Y(\mathrm{C78})$; Δ' values are for an "ideal solution" of group X. *Retention indices*: I_{130} is for the retention index at the reference temperature $T^{\dagger} = 130 + 273.15\mathrm{K}$; for the meaning of the coefficients, A, see Eq. (7). *Thermodynamic functions*: H and S are for partial molar enthalpy and entropy at $T^{\dagger}$, C_P is for the mean partial molar heat capacity in the temperature range indicated; for the meaning of the coefficients h and s see Eq. (6). At the end of the table additive corrections are listed *to convert data A*: to those related to the partition coefficients K_D; B: to those where pressures are measured in units of bar (instead of atm). *Errors*. The symbol σ is for the standard deviation around the regression and at the end of the table are listed standard deviations of constants and functions in units of the standard deviation around the regression, $f(\mathrm{coeff}) = \sigma(\mathrm{coeff})/\sigma$. Data marked by superscript, s, are significant at the 10% significance level if tested against σ. Data marked by one asterisk are at the 20% significance level, those marked by double asterisk are under this limit. Note that *linearity* of the following thermodynamic functions of *n-alkanes with carbon number* was imposed by the regression function: ΔH, ΔS, ΔC_P, h, s, $\Delta'H$, $\Delta'S$ and $\Delta'C_P$.

No.	*Compound*	*Temp. range*	*n*	*Retention index : C78 / TMO*								*σ*
				TMO- C78			*Mixture*		*id([OCH₃]=1) - C78*			
		(°C)		ΔI_{130}	10 x ΔA_T (K^{-1})	100x ΔA_{TT} (K^{-2})	A_L	10 x A_{LT} (K^{-1})	$\Delta' I_{130}$ (l mol⁻¹)	10 x $\Delta' A_T$ (K^{-1}l mol⁻¹)	100x $\Delta' A_{TT}$ (K^{-2}l mol⁻¹)	
HYDROCARBONS												
n-Alkanes												
00.05	Pentane	90-210	21									
00.06	Hexane	90-210	21									
00.07	Heptane	90-210	21									
00.08	Octane	90-210	21									
00.09	Nonane	90-210	21									
00.10	Decane	90-210	21									
00.11	Undecane	150-210	12									
00.12	Dodecane	150-210	12									
00.13	Tridecane	150-210	12									
00.14	Tetradecane	150-210	12									
Isoalkanes												
10.01	2,2-Dimethylbutane	90-170	15	+ 1.0	+0.16*		+ 1.0**	-0.08**	+ 0.7	+0.03		0.41
10.02	2,3-Dimethylbutane	90-170	15	+ 1.2	+0.20**		+ 0.1**	-0.04**	+ 0.5	+0.06		0.69
10.03	2,2-Dimethylpentane	90-170	15	+ 0.7	-0.02**		+ 0.9*	-0.22**	+ 0.5	-0.08		0.26
10.04	2,3-Dimethylpentane	90-170	15	+ 0.9	+0.09**		- 0.2**	-0.26**	+ 0.2	-0.06		0.33
10.05	2,4-Dimethylpentane	90-170	15	+ 0.2*	-0.16		+ 0.4*	-0.18**	+ 0.2	-0.12		0.23
10.06	2,2-Dimethylhexane	90-170	15	+ 0.4	-0.02**		+ 0.4**	-0.28**	+ 0.3	-0.10		0.35
10.07	2,3-Dimethylhexane	90-170	15	+ 0.9	+0.10**		- 0.4**	-0.09**	+ 0.2	+0.01		0.32
10.08	2,4-Dimethylhexane	90-170	15	- 0.1**	+0.03**		- 0.3**	+0.16**	- 0.1	+0.06		0.27
10.09	3,4-Dimethylhexane	90-170	15	+ 1.0	+0.05**		- 0.4**	+0.23**	+ 0.2	+0.10		0.34
10.10	2,2,3-Trimethylbutane	90-170	15	+ 1.3	+0.48		+ 0.1**	+0.84	+ 0.5	+0.46		0.35

No.	*Thermodynamic data : C78 / TMO*								
	TMO- C78			*Mixture*		*id([OCH_3]=1) - C78*			*σ*
	ΔH (cal mol^{-1})	*ΔS* (cal $mol^{-1}K^{-1}$)	*$ΔC_P$* (cal $mol^{-1}K^{-1}$)	*h* (cal mol^{-1})	*s* (cal mol^{-1} K^{-1})	*ΔH* (cal l mol^{-2})	*ΔS* (cal l $mol^{-2}K^{-1}$)	*$ΔC_P$* (cal l $mol^{-2}K^{-1}$)	(cal mol^{-1})
HYDROCARBONS									
n-Alkanes									
00.05	+ 22	-0.103	+ 1.1	- 162	-0.489	- 59	-0.230	+0.2	6.6
00.06	+ 12	-0.139	+ 1.2	- 155	-0.489	- 61	-0.245	+0.3	5.6
00.07	+ 1	-0.176	+ 1.4	- 148	-0.489	- 64	-0.261	+0.3	4.2
00.08	- 10	-0.213	+ 1.5	- 142	-0.489	- 66	-0.276	+0.3	2.6
00.09	- 20	-0.249	+ 1.7	- 135	-0.489	- 69	-0.291	+0.4	3.4
00.10	- 31	-0.286	+ 1.8	- 129	-0.489	- 71	-0.307	+0.4	4.5
00.11	- 42	-0.323	+ 1.9	- 122	-0.489	- 74	-0.322	+0.5	5.9
00.12	- 52	-0.359	+ 2.1	- 115	-0.489	- 76	-0.338	+0.5	5.5
00.13	- 63	-0.396	+ 2.2	- 109	-0.489	- 79	-0.353	+0.5	6.6
00.14	- 74	-0.432	+ 2.4	- 102	-0.489	- 81	-0.368	+0.6	6.9
Isoalkanes									
10.01	+ 44^{s}	-0.043**	+ 2.4*	- 190	-0.552	- 60	-0.229	+0.7	2.2
10.02	+ 49*	-0.035**	+ 4.2*	- 170*	-0.521^{s}	- 52	-0.217	+1.3	3.3
10.03	- 4**	-0.172	+ 1.6*	- 214	-0.627	- 86	-0.302	+0.4	1.4
10.04	+ 12**	-0.137	+ 2.2*	- 204	-0.625	- 78	-0.292	+0.6	1.8
10.05	- 29	-0.238	+ 1.1**	- 200	-0.599	- 90	-0.317	+0.2	1.2
10.06	- 11**	-0.202	+ 1.1**	- 212	-0.645	- 89	-0.323	+0.2	2.0
10.07	+ 4**	-0.166	+ 1.9**	- 159	-0.532	- 67	-0.273	+0.5	1.8
10.08	+ 4**	-0.174	+ 1.7*	- 111	-0.407	- 50	-0.233	+0.4	1.5
10.09	- 9**	-0.199	+ 3.0	- 91*	-0.366	- 48	-0.227	+0.9	1.6
10.10	+ 93	+0.071*	+ 1.9*	+ 22**	-0.059**	+ 28	-0.025	+0.6	1.7

(Continued on pages 398 and 399)

Table 8 (*continued*)

No.	Compound	Temp. range (°C)	n	Retention index : C78 / TMO: TMO-C78 ΔI_{130}	$10\times\Delta A_T$ (K^{-1})	$100\times\Delta A_{TT}$ (K^{-2})	Mixture A_L	$10\times A_{LT}$ (K^{-1})	id([OCH_3]=1) - C78 $\Delta' I_{130}$ ($l\ mol^{-1}$)	$10\times\Delta' A_T$ ($K^{-1} l\ mol^{-1}$)	$100\times\Delta' A_{TT}$ ($K^{-2} l\ mol^{-1}$)	σ
10.11	2,2,4-Trimethylpentane	90-170	15	+ 0.0**	+0.43		+ 0.5**	+0.17**	+ 0.2	+0.21		0.41
10.12	2,3,4-Trimethylpentane	90-170	15	+ 1.3	+0.30		+ 0.0**	+0.57	+ 0.5	+0.30		0.25
1-Alkenes												
11.05	1-Pentene	90-170	15	+ 6.3	-0.10**		- 2.2	-0.75	+ 1.4	-0.28		0.43
11.06	1-Hexene	90-170	15	+ 7.4	-0.14		+ 0.4**	-0.91	+ 2.7	-0.34		0.21
11.07	1-Heptene	90-170	15	+ 8.2	-0.01**		+ 1.5	-0.53	+ 3.3	-0.16		0.24
11.08	1-Octene	90-170	15	+ 7.8	-0.13		+ 0.9	-0.18	+ 3.0	-0.08		0.14
11.09	1-Nonene	90-170	15	+ 7.8	-0.04**		+ 2.2	-0.14**	+ 3.5	-0.03		0.16
11.10	1-Decene	90-170	15	+ 7.7	-0.02**		+ 1.6	-0.15**	+ 3.2	-0.03		0.19
1-Alkynes												
12.05	1-Pentyne	90-170	15	+ 30.5	-0.12**		+ 8.5	+0.39**	+13.5	+0.21		0.38
12.06	1-Hexyne	90-170	15	+ 31.2	-0.20[s]		+ 9.7	+0.18**	+14.1	+0.11		0.40
12.07	1-Heptyne	90-170	15	+ 32.1	-0.03**		+10.4	+0.38*	+14.7	+0.24		0.34
12.08	1-Octyne	90-170	15	+ 31.8	-0.11**		+ 9.3	+0.24**	+14.2	+0.16		0.43
12.09	1-Nonyne	90-170	15	+ 31.9	-0.20		+ 9.1	+0.20**	+14.2	+0.12		0.32
12.10	1-Decyne	90-170	15	+ 31.8	-0.09**		+ 9.5	+0.13**	+14.3	+0.13		0.37
Alkynes												
13.01	2-Hexyne	90-170	15	+ 23.0	-0.16		+ 5.7	-0.63	+ 9.9	-0.19		0.20
13.02	3-Hexyne	90-170	15	+ 21.7	-0.24		+ 6.3	-0.46*	+ 9.7	-0.16		0.36
13.03	4-Octyne	90-170	15	+ 19.8	-0.15*		+ 5.4	-0.15**	+ 8.7	-0.03		0.36
Monocyclic hydrocarbons												
14.05	Cyclopentane	90-170	15	+ 3.0	+0.06**		- 0.3**	-0.36	+ 0.9	-0.10		0.87
14.06	Cyclohexane	90-170	15	+ 2.7	+0.36*		- 0.6**	+0.45**	+ 0.7	+0.29		0.92
14.07	Cycloheptane	90-170	15	+ 3.0	+0.58		+ 0.0**	+0.35**	+ 1.1	+0.33		0.78
14.08	Cyclooctane	90-170	15	+ 4.0	+0.61		- 0.5**	+1.17*	+ 1.3	+0.63		0.88
14.10	Cyclodecane	130-210	15	+ 6.7	-0.06**		+ 3.6[s]	-0.51**	+ 3.6	-0.17		0.49
Bicyclic hydrocarbons												
15.01	*cis*-Hydrindane	130-210	15	+ 4.6	+0.06**		- 0.6**	+0.29**	+ 1.4	+0.13		0.92
15.02	*trans*-Hydrindane	130-210	15	+ 3.7	+0.27**		- 2.4**	+0.66**	+ 0.5	+0.33		0.91
15.03	*cis*-Decalin	130-210	15	+ 5.5	+0.20**		+ 4.4**	-0.11**	+ 3.4	+0.06		0.91
15.04	*trans*-Decalin	130-210	15	+ 4.1	-0.04**		- 0.0**	-0.06**	+ 1.4	-0.02		0.58

No.	Thermodynamic data : C78 / TMO								
	TMO- C78			Mixture		id([OCH_3]=1) - C78			σ
	ΔH (cal mol^{-1})	ΔS (cal $mol^{-1}K^{-1}$)	ΔC_P (cal $mol^{-1}K^{-1}$)	$\tilde{h}$ (cal mol^{-1})	s (cal mol^{-1} K^{-1})	$\Delta' H$ (cal l mol^{-2})	$\Delta' S$ (cal l $mol^{-2}K^{-1}$)	$\Delta' C_P$ (cal l $mol^{-2}K^{-1}$)	(cal mol^{-1})
10.11	+ 88	+0.044**	- 1.0**	- 120*	-0.413	- 24	-0.159	-0.4	2.2
10.12	+ 41	-0.071	+ 2.5	- 28**	-0.203	- 9	-0.126	+0.8	1.0
1-Alkenes									
11.05	- 59	-0.223	+ 3.7[s]	- 308	-0.880	- 134	-0.398	+1.0	2.1
11.06	- 93	-0.294	+ 0.6**	- 370	-1.012	- 166	-0.466	-0.1	1.4
11.07	- 82	-0.277	+ 3.0	- 277	-0.785	- 130	-0.383	+0.8	0.9
11.08	- 114	-0.373	+ 2.5[s]	- 186	-0.585	- 112	-0.351	+0.6	0.7
11.09	- 106	-0.366	+ 2.7	- 186	-0.583	- 110	-0.349	+0.7	0.8
11.10	- 112	-0.388	+ 0.8**	- 179	-0.592	- 111	-0.365	+0.0	0.9
1-Alkynes									
12.05	- 308	-0.504	+ 3.1[s]	- 156[s]	-0.355[s]	- 146	-0.262	+0.9	2.1
12.06	- 346	-0.616	+ 4.0	- 212	-0.482	- 179	-0.345	+1.2	1.8
12.07	- 329	-0.585	+ 3.4	- 174	-0.414	- 161	-0.315	+1.0	1.7
12.08	- 355	-0.669	+ 3.7[s]	- 182	-0.465	- 175	-0.367	+1.0	2.1
12.09	- 386	-0.756	+ 2.5*	- 185	-0.495	- 189	-0.411	+0.6	1.9
12.10	- 373	-0.742	+ 3.9	- 191	-0.521	- 187	-0.418	+1.1	2.0
Alkynes									
13.01	- 261	-0.522	+ 2.0	- 338	-0.873	- 202	-0.469	+0.4	1.0
13.02	- 264	-0.539	- 0.0**	- 309	-0.790	- 193	-0.447	-0.3	0.8
13.03	- 245	-0.544	+ 0.1**	- 221	-0.618	- 160	-0.400	-0.2	0.8
Monocyclic hydrocarbons									
14.05	- 4**	-0.149[s]	+ 5.9[s]	- 238[s]	-0.694	- 93	-0.314	+1.8	3.4
14.06	+ 45**	-0.042**	+ 4.7*	- 59**	-0.276**	- 17	-0.138	+1.5	3.8
14.07	+ 68*	+0.011**	+ 2.2**	- 84**	-0.353**	- 18	-0.149	+0.7	3.9
14.08	+ 48*	-0.041**	+ 4.4*	+ 99**	+0.072**	+ 37	-0.024	+1.5	3.8
14.10	- 215	-0.673	+ 3.9[s]	- 252	-0.782	- 173	-0.531	+1.0	2.0
Bicyclic hydrocarbons									
15.01	- 190**	-0.620[s]	+ 4.6**	- 78**	-0.379**	- 106	-0.378	+1.3	4.6
15.02	- 28**	-0.232**	+ 1.7**	- 3**	-0.207**	- 26	-0.189	+0.5	4.6
15.03	- 222*	-0.699[s]	+ 5.5*	- 191**	-0.616[s]	- 154	-0.481	+1.6	4.1
15.04	- 252	-0.787	+ 5.7	- 146	-0.553	- 151	-0.496	+1.6	1.6

(Continued on pages 400 and 401)

Table 8 (*continued*)

No.	Compound	Temp. range (°C)	n	Retention index : C78 / TMO: TMO- C78 ΔI_{130}	$10\times \Delta A_T$ (K^{-1})	$100\times \Delta A_{TT}$ (K^{-2})	Mixture A_L	$10\times A_{LT}$ (K^{-1})	id([OCH_3]=1) - C78 δI_{130} (l mol^{-1})	$10\times \delta A_T$ (K^{-1}l mol^{-1})	$100\times \delta A_{TT}$ (K^{-2}l mol^{-1})	σ
Methylcyclohexanes (MCH)												
16.01	Methylcyclohexane	90-170	15	+ 2.3	+0.14**		- 1.8	+0.34**	+ 0.2	+0.17		0.34
16.02	*cis*-1,2-Di MCH	90-170	15	+ 2.8	+0.12**		- 0.0**	+0.34**	+ 0.8	+0.17		0.55
16.03	*trans*-1,2-Di MCH	90-170	15	+ 2.2	+0.18*		- 0.5**	+0.20**	+ 0.6	+0.14		0.53
16.04	*cis*-1,4-Di MCH	90-170	15	+ 2.6	+0.08**		+ 0.4**	+0.23**	+ 1.0	+0.12		0.27
16.05	*trans*-1,4-Di MCH	90-170	15	+ 2.4	+0.24*		+ 0.1**	+0.15**	+ 0.9	+0.14		0.59
Cyclohexenes												
17.01	Cyclohexene	90-170	15	+ 9.6	+0.14*		+ 1.6^{s}	+0.40**	+ 3.9	+0.22		0.40
17.02	1,3-Cyclohexadiene	90-170	15	+ 18.4	+0.29^{s}		+ 4.2	+0.65*	+ 7.8	+0.39		0.60
17.03	1,4-Cyclohexadiene	90-170	15	+ 18.8	+0.28**		+ 4.6^{s}	+0.19**	+ 8.1	+0.23		0.98
Alkylbenzenes												
18.00	Benzene	90-170	15	+ 28.9	+0.46		+ 8.2	+0.79	+12.9	+0.54		0.39
18.01	Toluene	90-170	15	+ 27.9	+0.41		+ 7.2	+0.80	+12.2	+0.52		0.38
18.02	Ethylbenzene	90-170	15	+ 27.5	+0.30		+ 7.6	+0.80	+12.2	+0.48		0.48
Miscellaneous												
19.01	Adamantane	130-210	15	+ 5.7	+0.59		+ 0.4**	+0.47*	+ 2.1	+0.38		0.36
19.02	Naphthalene	130-210	15	+ 47.9	+0.19**		+18.3	-0.51**	+22.9	+0.08		0.75
19.03	Azulene	130-210	15	+ 56.4	-0.77**	+0.23	+18.3	+1.42	+25.8	+0.45	+0.08	0.71
ALKANE DERIVATIVES												
1-Fluoroalkanes												
20.05	1-Fluoropentane	90-170	15	+ 27.4	-0.20*		+10.1	-0.46**	+12.9	-0.12		0.52
20.06	1-Fluorohexane	90-170	15	+ 27.7	-0.16*		+11.0	-0.06**	+13.4	+0.03		0.43
20.07	1-Fluoroheptane	90-170	15	+ 27.8	-0.21*		+12.6	+0.31**	+13.9	+0.15		0.51
20.08	1-Fluorooctane	90-170	15	+ 28.3	-0.17		+12.0	+0.23**	+13.9	+0.14		0.30
1,1,1-Trifluoroalkanes												
21.08	1,1,1-Trifluorooctane	90-170	15	+ 29.5	-0.45		+12.1	-0.19*	+14.4	-0.10		0.15
21.10	1,1,1-Trifluorodecane	90-170	15	+ 29.6	-0.69		+11.9	-0.48	+14.3	-0.29		0.20
1-Chloroalkanes												
22.04	1-Chlorobutane	90-170	15	+ 30.1	+0.04**		+11.1	-0.27**	+14.2	+0.04		0.77

No.	Thermodynamic data : C78 / TMO								
	TMO- C78			Mixture		id([OCH_3]=1) - C78			σ
	ΔH	ΔS	ΔCp	h	s	Δ'H	Δ'S	Δ'Cp	
	(cal mol^{-1})	(cal mol^{-1}K^{-1})		(cal mol^{-1})	(cal mol^{-1} K^{-1})	(cal l mol^{-2})	(cal l mol^{-2}K^{-1})		(cal mol^{-1})
Methylcyclohexanes (MCH)									
16.01	- 4**	-0.168	+ 2.0*	- 69*	-0.326	- 39	-0.203	+0.6	1.4
16.02	- 26	-0.227	+ 2.8	- 78	-0.343	- 49	-0.229	+0.8	2.8
16.03	- 3**	-0.177	+ 2.9*	- 101**	-0.401^{s}	- 49	-0.232	+0.9	2.7
16.04	- 30^{s}	-0.235	+ 1.9*	- 103^{s}	-0.395	- 59	-0.248	+0.5	1.5
16.05	+ 10**	-0.143	+ 3.9^{s}	- 119*	-0.435^{s}	- 50	-0.230	+1.2	2.5
Cyclohexenes									
17.01	- 74	-0.245	+ 2.8^{s}	- 94*	-0.335	- 65	-0.216	+0.8	1.7
17.02	- 138	-0.291	+ 4.4^{s}	- 60**	-0.216**	- 68	-0.174	+1.4	2.5
17.03	- 135	-0.289	+ 6.3^{s}	- 152**	-0.443**	- 98	-0.251	+2.0	4.5
Alkylbenzenes									
18.00	- 209	-0.324	+ 2.3**	- 60**	-0.159**	- 84	-0.145	+0.7	2.2
18.01	- 219	-0.380	+ 1.7**	- 53**	-0.175**	- 88	-0.177	+0.5	2.2
18.02	- 246	-0.461	+ 1.4**	- 47**	-0.170**	- 96	-0.206	+0.3	2.7
Miscellaneous									
19.01	+ 34**	-0.071**	+ 0.5**	- 70**	-0.359	- 27	-0.185	+0.1	1.8
19.02	- 604	-1.134	+ 4.7*	- 391	-0.949	- 324	-0.672	+1.2	3.6
19.03	- 793	-1.516	+11.3	- 71**	-0.171**	- 275	-0.526	+3.5	3.2
ALKANE DERIVATIVES									
1-Fluoroalkanes									
20.05	- 303	-0.543	+ 4.3	- 362	-0.856	- 217	-0.452	+1.2	2.1
20.06	- 310	-0.590	+ 4.4	- 276	-0.654	- 191	-0.403	+1.3	1.5
20.07	- 326	-0.647	+ 4.5	- 203	-0.473	- 173	-0.362	+1.3	2.1
20.08	- 339	-0.683	+ 3.1	- 211	-0.518	- 181	-0.394	+0.8	1.5
1,1,1-Trifluroalkanes									
21.08	- 388	-0.769	+ 3.1	- 399	-0.709	- 226	-0.483	+0.8	0.7
21.10	- 461	-0.974	+ 1.9	- 344	-0.860	- 270	-0.612	+0.3	1.0
1-Chloroalkanes									
22.04	- 292	-0.518	+ 5.8^{s}	- 322	-0.765	- 200	-0.413	+1.7	3.3

(Continued on pages 402 and 403)

Table 8 (*continued*)

No.	*Compound*	*Temp. range* ($^{\circ}C$)	*n*	*Retention index : C78 / TMO*								
				TMO- C78			*Mixture*		*id([OCH_3]=1) - C78*			σ
				ΔI_{130}	$10\times$ ΔA_T (K^{-1})	$100\times$ ΔA_{TT} (K^{-2})	A_L	$10\times$ A_{LT} (K^{-1})	$\Delta' I_{130}$ ($l\ mol^{-1}$)	$10\times$ $\Delta' A_T$ ($K^{-1} l\ mol^{-1}$)	$100\times$ $\Delta' A_{TT}$ ($K^{-2} l\ mol^{-1}$)	
22.05	1-Chloropentane	90-170	15	+ 29.8	+0.36^{s}		+11.1	+0.77**	+14.2	+0.51		0.74
22.06	1-Chlorohexane	90-170	15	+ 30.1	+0.17**		+11.2	+0.79*	+14.3	+0.45		0.71
1-Bromoalkanes												
23.03	1-Bromopropane	90-170	15	+ 31.6	+0.13*		+11.8	+0.35**	+15.0	+0.29		0.34
23.04	1-Bromobutane	90-170	15	+ 30.8	+0.07**		+11.0	+0.38*	+14.5	+0.28		0.31
23.05	1-Bromopentane	90-170	15	+ 30.9	+0.07**		+10.7	+0.62	+14.4	+0.36		0.26
1-Cyanoalkanes												
24.02	Cyanoethane	90-170	15	+ 85.2	-0.67		+40.5	-0.13**	+43.5	+0.08		1.23
24.03	1-Cyanopropane	90-170	15	+ 82.4	-0.43		+40.5	-0.19**	+42.5	+0.14		0.66
24.04	1-Cyanobutane	90-170	15	+ 81.8	-0.25*		+40.5	+0.08**	+42.3	+0.29		0.61
24.05	1-Cyanopentane	90-170	15	+ 82.3	-0.24*		+41.5	+0.36**	+42.8	+0.40		0.65
1-Nitroalkanes												
25.02	Nitroethane	90-170	15	+ 92.4	-0.79		+41.2	-0.77	+46.2	-0.16		0.36
25.03	1-Nitropropane	90-170	15	+ 86.8	-0.64		+38.9	-0.43**	+43.5	-0.01		0.45
25.04	1-Nitrobutane	90-170	15	+ 84.9	-0.65		+37.7	-0.15**	+42.4	+0.07		0.39
25.05	1-Nitropentane	90-170	15	+ 84.5	-0.59		+38.6	-0.21**	+42.6	+0.08		0.43
1-Acetoxyalkanes												
26.03	1-Acetoxypropane	90-170	15	+ 45.9	-0.17^{s}		+19.5	-0.14**	+22.6	+0.08		0.39
26.04	1-Acetoxybutane	90-170	15	+ 46.0	-0.11**		+19.3	+0.00**	+22.6	+0.15		0.47
26.05	1-Acetoxypentane	90-170	15	+ 46.3	-0.17*		+19.6	-0.09**	+22.8	+0.10		0.44
1-Alkanols												
27.04	1-Butanol	90-170	15	+ 97.8	-3.58	+0.15	+48.6	-3.58	+50.6	-2.05	+0.03	0.51
27.05	1-Pentanol	90-170	15	+ 99.6	-3.49	+0.19	+49.4	-3.25	+51.5	-1.89	+0.05	0.36
27.06	1-Hexanol	90-170	15	+101.3	-3.68	+0.15	+50.6	-3.37	+52.5	-1.99	+0.04	0.42
27.07	1-Heptanol	90-170	15	+102.3	-3.47	+0.13	+51.3	-3.47	+53.1	-1.96	+0.03	0.45
2-Alkanols												
28.04	2-Butanol	90-170	15	+ 81.9	-3.01	+0.15	+37.6	-2.58	+41.3	-1.59	+0.04	0.37
28.05	2-Pentanol	90-170	15	+ 83.0	-2.80	+0.14	+38.9	-2.26	+42.1	-1.39	+0.04	0.35
28.06	2-Hexanol	90-170	15	+ 84.3	-2.96	+0.14	+39.8	-2.14	+42.9	-1.40	+0.04	0.32
28.07	2-Heptanol	90-170	15	+ 85.3	-2.99	+0.14	+41.2	-2.47	+43.7	-1.52	+0.04	0.41

No.	Thermodynamic data : C78 / TMO								
	TMO- C78			Mixture		id([OCH$_3$]=1) - C78			σ
	ΔH (cal mol^{-1})	ΔS (cal mol^{-1}K^{-1})	ΔC_P (cal mol^{-1}K^{-1})	h (cal mol^{-1})	s (cal mol^{-1} K^{-1})	$\Delta' H$ (cal l mol^{-2})	$\Delta' S$ (cal l mol^{-2}K^{-1})	$\Delta' C_P$ (cal l mol^{-2}K^{-1})	(cal mol^{-1})
22.05	- 231	-0.385	+ 5.1^{s}	- 97**	-0.227**	- 103	-0.186	+1.6	2.9
22.06	- 289	-0.539	+ 4.8^{s}	- 91**	-0.232**	- 122	-0.244	+1.5	3.1
1-Bromoalkanes									
23.03	- 291	-0.488	+ 3.9	- 203	-0.459	- 157	-0.294	+1.2	1.3
23.04	- 302	-0.544	+ 3.5	- 180	-0.433	- 156	-0.311	+1.0	1.1
23.05	- 319	-0.598	+ 3.1	- 123	-0.315	- 143	-0.293	+0.9	1.3
1-Cyanoalkanes									
24.02	- 980	-1.432	+10.7	- 588	-0.986	- 473	-0.667	+3.2	4.8
24.03	- 932	-1.413	+ 6.9	- 631	-1.118	- 477	-0.721	+1.9	2.8
24.04	- 883	-1.334	+ 5.6	- 544	-0.949	- 435	-0.646	+1.5	2.9
24.05	- 904	-1.406	+ 6.3	- 489	-0.825	- 424	-0.632	+1.8	3.0
1-Nitroalkanes									
25.02	-1 114	-1.705	+ 3.4^{s}	- 760	-1.389	- 575	-0.894	+0.6	2.1
25.03	-1 019	-1.589	+ 3.4*	- 653	-1.217	- 516	-0.818	+0.6	2.7
25.04	-1 011	-1.622	+ 3.4^{s}	- 555	-1.020	- 484	-0.772	+0.7	2.3
25.05	-1 008	-1.637	+ 2.3**	- 581	-1.099	- 493	-0.809	+0.3	2.5
1-Acetoxyalkanes									
26.03	- 496	-0.812	+ 3.6^{s}	- 373	-0.782	- 274	-0.486	+0.9	2.3
26.04	- 490	-0.814	+ 2.5**	- 332	-0.704	- 259	-0.464	+0.6	2.8
26.05	- 523	-0.906	+ 1.6**	- 349	-0.763	- 278	-0.519	+0.2	2.5
1-Alkanols									
27.04	-1 759	-3.263	+13.9	-1 436	-3.014	-1 024	-1.974	+3.5	3.3
27.05	-1 737	-3.222	+14.3	-1 331	-2.781	- 982	-1.884	+3.7	2.4
27.06	-1 806	-3.400	+13.8	-1 360	-2.864	-1 017	-1.976	+3.5	2.8
27.07	-1 775	-3.327	+12.4	-1 364	-2.886	-1 008	-1.960	+3.0	2.7
2-Alkanols									
28.04	-1 461	-2.684	+12.4	-1 151	-2.378	- 834	-1.582	+3.2	2.1
28.05	-1 427	-2.647	+11.9	-1 047	-2.185	- 791	-1.515	+3.1	2.3
28.06	-1 475	-2.776	+11.9	- 987	-2.053	- 789	-1.517	+3.1	1.8
28.07	-1 502	-2.852	+12.3	-1 074	-2.277	- 828	-1.622	+3.2	2.5

(*Continued on pages 404 and 405*)

Table 8 (*continued*)

No.	Compound	Temp. range	n	Retention index : C78 / TMO								
				TMO- C78			Mixture		id([OCH_3]=1) - C78			σ
		(°C)		ΔI_{130}	10 × ΔA_T (K^{-1})	100× ΔA_{TT} (K^{-2})	A_L	10 × A_{LT} (K^{-1})	ΔI_{130} (l mol^{-1})	10 × ΔA_T (K^{-1}l mol^{-1})	100× ΔA_{TT} (K^{-2}l mol^{-1})	
2-Methyl-2-alkanols												
29.04	2-Methyl-2-propanol	90-170	15	+ 74.2	-2.91	+0.17	+33.6	-3.01	+37.3	-1.73	+0.04	0.51
29.05	2-Methyl-2-butanol	90-170	15	+ 72.3	-2.75	+0.13	+34.6	-2.44	+36.9	-1.48	+0.03	0.47
29.06	2-Methyl-2-pentanol	90-170	15	+ 72.1	-2.68	+0.15	+34.7	-2.07	+36.9	-1.33	+0.04	0.42
29.07	2-Methyl-2-hexanol	90-170	15	+ 72.7	-2.78	+0.14	+34.5	-2.17	+37.1	-1.40	+0.04	0.42
1-Alkanethiols												
30.04	1-Butanethiol	90-170	15	+ 30.1	-0.83		+10.1	-1.23	+13.9	-0.59		0.32
30.05	1-Pentanethiol	90-170	15	+ 30.2	-0.80		+10.1	-1.18	+13.9	-0.57		0.32
30.06	1-Hexanethiol	90-170	15	+ 30.5	-0.70		+10.2	-1.25	+14.0	-0.56		0.41
2-Alkanones												
31.04	2-Butanone	90-170	15	+ 52.6	-0.59		+22.0	-1.32	+25.8	-0.45		0.26
31.05	2-Pentanone	90-170	15	+ 52.1	-0.38		+24.4	-0.78	+26.8	-0.18		0.20
31.06	2-Hexanone	90-170	15	+ 52.8	-0.34		+25.2	-0.36^{s}	+26.9	-0.02		0.22
31.07	2-Heptanone	90-170	15	+ 53.3	-0.36		+25.9	-0.33*	+27.4	-0.01		0.23
Aldehydes												
32.05	Pentanal	90-170	15	+ 49.2	-0.88		+22.7	-1.61	+24.8	-0.66		0.31
32.06	Hexanal	90-170	15	+ 50.3	-0.78		+22.6	-0.55**	+25.2	-0.25		0.53
32.07	Heptanal	90-170	15	+ 50.8	-0.51		+23.0	-0.53	+25.5	-0.15		0.29
Ethers												
33.06	Dipropylether	90-170	15	+ 15.1	-0.23		+ 6.6	-0.64	+ 7.5	-0.24		0.24
33.08	Dibutylether	90-170	15	+ 14.8	-0.15		+ 6.6	-0.36	+ 7.4	-0.12		0.21
Halomethanes												
37.01	Dichloromethane	90-170	15	+ 59.3	-0.78		+21.5	+0.21**	+27.9	+0.03		0.39
37.02	Trichloromethane	90-170	15	+ 65.2	-1.52		+23.5	-0.69*	+30.6	-0.51		0.50
37.03	Tetrachloromethane	90-170	15	+ 19.7	-0.34		+ 2.6	+0.21^{s}	+ 7.7	+0.02		0.13
37.04	CF_2Br_2	90-170	15	+ 24.8	-0.59		+ 3.8	-1.04	+ 9.9	-0.48		0.49
HALOBENZENES												
38.01	Fluorobenzene	90-170	15	+ 39.9	-0.04**		+12.2	+0.10**	+18.0	+0.17		0.33
38.02	Hexafluorobenzene	90-170	15	+ 36.9	-0.66		+15.2	-0.58^{s}	+17.9	-0.28		0.41
38.03	Trifluoromethylbenzene	90-170	15	+ 46.9	-0.24		+16.4	+0.16**	+21.9	+0.15		0.33

No.	Thermodynamic data : C78 / TMO								
	TMO- C78			Mixture		id([OCH$_3$]=1) - C78			σ
	ΔH (cal mol^{-1})	ΔS (cal mol^{-1}K^{-1})	ΔC$_P$ (cal mol^{-1}K^{-1})	h (cal mol^{-1})	s (cal mol^{-1} K^{-1})	Δ'H (cal l mol^{-2})	Δ'S (cal l mol^{-2}K^{-1})	Δ'C$_P$ (cal l mol^{-2}K^{-1})	(cal mol^{-1})
2-Methyl-2-alkanols									
29.04	-1 383	-2.562	+12.6	-1 175	-2.526	- 822	-1.608	+3.3	3.0
29.05	-1 326	-2.523	+11.8	-1 049	-2.244	- 765	-1.512	+3.1	2.8
29.06	-1 294	-2.468	+11.6	- 937	-1.991	- 718	-1.412	+3.1	2.4
29.07	-1 330	-2.573	+11.9	- 941	-2.023	- 733	-1.463	+3.2	2.4
1-Alkanethiols									
30.04	- 480	-0.991	+ 3.6	- 506	-1.248	- 330	-0.746	+0.8	1.7
30.05	- 489	-1.028	+ 4.3	- 489	-1.224	- 328	-0.754	+1.0	1.6
30.06	- 478	-1.011	+ 4.7	- 496	-1.255	- 328	-0.761	+1.1	1.8
2-Alkanones									
31.04	- 646	-1.039	+ 2.0*	- 676	-1.463	- 420	-0.775	+0.2	1.7
31.05	- 606	-1.001	+ 2.3	- 566	-1.193	- 371	-0.676	+0.4	1.2
31.06	- 609	-1.018	+ 1.4*	- 472	-0.973	- 341	-0.609	+0.1	1.2
31.07	- 634	-1.093	+ 1.7*	- 471	-0.982	- 350	-0.641	+0.2	1.2
Aldehydes									
32.05	- 675	-1.163	+ 3.9	- 745	-1.625	- 455	-0.877	+0.8	1.7
32.06	- 670	-1.195	+ 7.2	- 495	-1.045	- 371	-0.697	+2.0	1.5
32.07	- 624	-1.089	+ 3.8	- 484	-1.033	- 353	-0.660	+0.9	1.4
Ethers									
33.06	- 196	-0.469	+ 3.4	- 351	-0.898	- 188	-0.469	+0.9	0.9
33.08	- 198	-0.499	+ 1.3*	- 276	-0.747	- 166	-0.436	+0.2	0.9
Halomethanes									
37.01	- 753	-1.209	+ 2.0**	- 329	-0.608	- 334	-0.530	+0.3	2.4
37.02	- 979	-1.762	+ 7.1	- 547	-1.154	- 485	-0.905	+1.9	2.0
37.03	- 280	-0.616	+ 1.6	- 134	-0.416	- 142	-0.355	+0.3	0.7
37.04	- 358	-0.707	+ 4.2**	- 429	-1.094	- 263	-0.601	+1.1	2.7
HALOBENZENES									
38.01	- 422	-0.709	+ 3.8	- 245	-0.561	- 212	-0.394	+1.1	1.2
38.02	- 499	-0.895	+ 4.2	- 431	-0.953	- 299	-0.584	+1.1	2.1
38.03	- 523	-0.872	+ 4.7	- 278	-0.589	- 252	-0.443	+1.3	1.4

(Continued on pages 406 and 407)

Table 8 (*continued*)

No.	*Compound*	*Temp. range* (°C)	*n*	*Retention index : C78 / TMO*								
				TMO- C78			*Mixture*		*id([OCH$_3$]=1) - C78*			*σ*
				ΔI_{130}	10 × ΔA_T (K^{-1})	100× ΔA_{TT} (K^{-2})	A_L	10 × A_{LT} (K^{-1})	$\Delta I'_{130}$ ($l\ mol^{-1}$)	10 × $\Delta A'_T$ ($K^{-1} l\ mol^{-1}$)	100× $\Delta A'_{TT}$ ($K^{-2} l\ mol^{-1}$)	
38.04	Chlorobenzene	90-170	15	+ 40.6	+0.01**		+11.7	+0.23**	+18.1	+0.23		0.59
38.05	Bromobenzene	90-170	15	+ 42.9	-0.03**		+12.9	+0.30**	+19.3	+0.25		0.43
38.06	Iodobenzene	130-210	15	+ 46.3	+0.26$		+13.0	+0.54**	+20.5	+0.45		0.57
ALKYLPYRIDINES												
39.01	Pyridine	90-170	15	+ 56.6	-0.24		+28.5	+0.15**	+29.4	+0.21		0.31
39.02	2-Picoline	90-170	15	+ 48.3	+0.09**		+25.1	+0.20**	+25.4	+0.31		0.30
39.03	3-Picoline	90-170	15	+ 56.4	+0.17*		+33.9	-0.23**	+31.2	+0.24		0.51
39.04	4-Picoline	90-170	15	+ 57.0	-0.03**		+34.4	-0.15**	+31.6	+0.20		0.29
39.05	2,3-Lutidine	130-210	15	+ 48.9	+0.42		+32.1	-1.02	+28.0	+0.02		0.32
39.06	2,4-Lutidine	130-210	15	+ 48.1	+0.49		+32.0	-0.48	+27.7	+0.23		0.27
39.07	2,5-Lutidine	130-210	15	+ 46.2	+0.53		+28.6	+0.07**	+25.9	+0.42		0.52
39.08	2,6-Lutidine	130-210	15	+ 42.3	-0.19**		+24.1	-1.17**	+22.9	-0.28		1.21
39.09	3,4-Lutidine	130-210	15	+ 60.5	-0.23		+45.2	-2.72	+36.5	-0.72		0.24
39.10	3,5-Lutidine	130-210	15	+ 56.5	-0.19		+40.6	-1.67	+33.5	-0.37		0.27
39.11	2-Ethylpyridine	130-210	15	+ 44.2	+0.11$		+25.8	-1.27	+24.2	-0.20		0.23
39.12	3-Ethylpyridine	130-210	15	+ 51.4	+0.01**		+28.2	-1.53	+27.5	-0.29		0.22
39.13	4-Ethylpyridine	130-210	15	+ 54.0	+0.05*		+32.6	-1.44	+29.9	-0.23		0.15
39.14	2-Propylpyridine	130-210	15	+ 42.9	+0.16**		+21.9	-1.56	+22.4	-0.30		0.60
39.15	4-Propylpyridine	130-210	15	+ 53.1	+0.75		+23.8	+1.20**	+26.6	+0.89		1.22
39.16	2,3,6-Collidine	130-210	15	+ 40.8	+0.19		+23.1	-0.87	+22.1	-0.05		0.24
39.17	2,4,6-Collidine	130-210	15	+ 41.5	-0.11		+25.4	-0.93	+23.1	-0.17		0.21
39.18	4-*tert*-Butylpyridine	130-210	15	+ 53.4	-0.02**		+38.7	-2.16	+31.8	-0.49		0.35
39.19	3-Chloropyridine	90-170	15	+ 57.6	-0.03**		+22.2	-0.06**	+27.6	+0.19		0.51
ORGANOSILICON COMPOUNDS												
40.01	Tetramethylsilane	90-170	15	+ 4.5	-0.16**		+ 0.7**	+0.61**	+ 1.8	+0.17		0.96
40.02	Hexamethyldisilane	90-170	15	+ 2.5	-0.01**		+ 2.3$	-0.05**	+ 1.7	-0.01		0.55
40.03	Hexamethyldisiloxane	90-170	15	+ 4.9	-0.30		+ 2.4	-0.17**	+ 2.5	-0.14		0.35
MISCELLANEOUS												
41.01	Carbon disulphide	90-170	15	+ 11.7	-0.03**		- 0.4**	-0.47**	+ 3.9	-0.14		0.51
41.02	Tetramethyltin	90-170	15	+ 6.7	+0.43		+ 2.8	+0.73	+ 3.3	+0.43		0.22
41.03	Tetrahydrofuran	90-170	15	+ 31.2	-0.08**		+15.4	-0.28**	+16.1	-0.01		0.36

No.	Thermodynamic data : C78 / TMO									
	TMO- C78			Mixture		id([OCH3]=1) - C78			σ
	ΔH (cal mol⁻¹)	ΔS (cal mol⁻¹K⁻¹)	ΔCp	h (cal mol⁻¹)	s (cal mol⁻¹ K⁻¹)	Δ'H (cal l mol⁻²)	Δ'S (cal l mol⁻²K⁻¹)	Δ'Cp	(cal mol⁻¹)
38.04	- 439	-0.784	+ 5.8	- 211	-0.524	- 209	-0.414	+1.7	1.8
38.05	- 481	-0.866	+ 3.8	- 208	-0.518	- 222	-0.439	+1.0	1.9
38.06	- 601	-1.129	+ 5.5	- 178§	-0.461	- 252	-0.507	+1.6	2.2
ALKYLPYRIDINES									
39.01	- 626	-1.019	+ 4.5	- 399	-0.749	- 316	-0.524	+1.2	1.4
39.02	- 491	-0.806	+ 4.1	- 361	-0.716	- 266	-0.457	+1.1	1.3
39.03	- 564	-0.892	+ 4.8	- 529	-1.028	- 340	-0.572	+1.3	2.3
39.04	- 611	-0.996	+ 3.7	- 516	-0.989	- 351	-0.593	+0.9	1.5
39.05	- 446	-0.699	+ 2.2*	- 613	-1.283	- 336	-0.611	+0.4	1.5
39.06	- 469	-0.762	+ 3.2	- 522	-1.054	- 312	-0.553	+0.7	1.0
39.07	- 442	-0.718	+ 3.1*	- 396	-0.781	- 262	-0.451	+0.8	2.5
39.08	- 593	-1.131	+ 5.0**	- 579	-1.281	- 380	-0.773	+1.2	5.3
39.09	- 721	-1.244	+ 4.1	-1 006	-2.108	- 552	-1.049	+0.7	1.2
39.10	- 720	-1.284	+ 5.1	- 806	-1.656	- 487	-0.917	+1.2	0.9
39.11	- 493	-0.866	+ 3.1	- 601	-1.321	- 353	-0.694	+0.6	1.1
39.12	- 572	-0.979	+ 3.1	- 672	-1.477	- 400	-0.775	+0.6	1.2
39.13	- 610	-1.041	+ 3.6	- 699	-1.489	- 418	-0.791	+0.7	0.9
39.14	- 364	-0.582	+ 0.8**	- 598	-1.379	- 312	-0.628	-0.1	1.7
39.15	- 446	-0.661**	+ 2.7**	- 124**	-0.187**	- 171	-0.229	+0.8	6.4
39.16	- 397	-0.691	+ 2.4§	- 484	-1.087	- 285	-0.566	+0.5	1.3
39.17	- 502	-0.937	+ 3.6	- 525	-1.154	- 332	-0.668	+0.8	1.1
39.18	- 630	-1.116	+ 3.4§	- 864	-1.847	- 480	-0.937	+0.6	1.7
39.19	- 543	-0.830	+ 0.5**	- 367	-0.782	- 284	-0.484	-0.1	2.0
ORGANOSILICON COMPOUNDS									
40.01	- 49**	-0.212§	+ 2.3	- 26**	-0.134**	- 32	-0.135	+0.7	6.2
40.02	- 27**	-0.205	- 1.4**	- 186§	-0.551	- 84	-0.285	-0.7	2.6
40.03	- 90	-0.323	+ 0.6*	- 209	-0.589	- 110	-0.332	-0.0	1.9
MISCELLANEOUS									
41.01	- 131	-0.345	+ 2.9**	- 266	-0.767	- 141	-0.395	+0.7	2.9
41.02	+ 33	-0.001**	+ 1.4*	- 27**	-0.139*	- 5	-0.064	+0.4	1.2
41.03	- 331	-0.582	+ 0.4**	- 370	-0.824	- 226	-0.447	-0.1	1.4

(*Continued on pages 408 and 409*)

Table 8 (*continued*)

No.	*Compound*	*Temp. range* (°C)	*n*	*Retention index : C78 / TMO*								
				TMO- C78			*Mixture*		*id([OCH$_3$]=1) - C78*			σ
				ΔI_{130}	$10\times$ ΔA_T (K^{-1})	$100\times$ ΔA_{TT} (K^{-2})	A_L	$10\times$ A_{LT} (K^{-1})	ΔI_{130} (l mol^{-1})	$10\times$ ΔA_T ($K^{-1} l$ mol^{-1})	$100\times$ ΔA_{TT} ($K^{-2} l$ mol^{-1})	
41.04	1,4-Dioxane	90-170	15	+ 47.4	-0.07**		+19.4	-0.18**	+23.1	+0.11		0.24
41.05	Thiophene	90-170	15	+ 38.5	+0.47		+10.4	+1.59	+17.1	+0.85		0.39
41.06	Cyclopentanone	90-170	15	+ 62.8	-0.13*		+28.9	-0.24**	+31.7	+0.13		0.32
41.07	Cyclohexanone	90-170	15	+ 61.6	+0.45		+29.8	+0.62^{s}	+31.6	+0.63		0.36
41.08	Cyclohexanol	90-170	15	+ 89.6	-2.99	+0.16	+43.9	-2.81	+46.2	-1.62	+0.04	0.43
41.11	Nitrobenzene	130-210	15	+ 87.2	+0.05**		+35.2	-0.10**	+42.3	+0.33		0.88
41.12	Benzyl alcohol	130-210	15	+152.3	-4.70	+0.20	+78.2	-3.61	+79.7	-2.21	+0.05	0.69
41.13	2-Phenylethanol	130-210	15	+134.9	-4.93	+0.29	+58.9	-2.10	+67.0	-1.87	+0.08	0.63
41.14	Anisole	130-210	15	+ 48.1	-0.23		+17.6	+0.24**	+22.7	+0.19		0.31
41.15	Phenetole	130-210	15	+ 45.1	+0.07*		+14.1	+0.31	+20.5	+0.30		0.17

ERROR OF THE COEFFICIENTS (STANDARD DEVIATION)

f(n-alkanes	*90-210*	*def.*							
f(n-alkanes)	*150-210*	*def.*							
f(solutes)	*90-170*	*0.63*	*0.22*	*0.093*	*2.19*	*0.78*	*0.61*	*0.28*	*0.032*
f(solutes)	*130-210*	*0.98*	*0.22*	*0.093*	*2.19*	*0.77*	*0.82*	*0.27*	*0.032*

CONVERSIONS

A	*Data related to K_D*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*
B	*Data related to 1 bar*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*

Table 8 (*continued*)

No.	*Thermodynamic data : C78 / TMO*								
	TMO- C78			*Mixture*		*id([OCH₃]=1) - C78*			σ
	ΔH (cal mol^{-1})	ΔS (cal $mol^{-1}K^{-1}$)	ΔC_p	h (cal mol^{-1})	s (cal mol^{-1} K^{-1})	$\Delta' H$ (cal l mol^{-2})	$\Delta' S$ (cal l $mol^{-2}K^{-1}$)	$\Delta' C_p$	(cal mol^{-1})
41.04	- 507	-0.825	+ 3.0	- 383	-0.804	- 280	-0.496	+0.7	1.4
41.05	- 309	-0.450	+ 2.1**	+ 54**	+0.155**	- 72	-0.064	+0.7	2.1
41.06	- 677	-1.063	+ 1.3**	- 473	-0.929	- 276	-0.249	+0.6	1.7
41.07	- 566	-0.828	+ 2.9*	- 311	-0.541	- 266	-0.382	+0.7	2.0
41.08	-1 560	-2.942	+12.9	-1 184	-2.516	- 882	-1.725	+3.3	2.6
41.11	-1 150	-1.976	+ 8.8	- 486	-0.945	- 511	-0.877	+2.5	2.9
41.12	-2 514	-4.559	+16.5	-1 418	-2.716	-1 240	-2.226	+4.2	3.8
41.13	-2 367	-4.423	+17.8	-1 035	-2.018	-1 079	-1.990	+4.8	2.8
41.14	- 564	-0.998	+ 2.3*	- 263	-0.588	- 264	-0.494	+0.5	1.7
41.15	- 483	-0.844	+ 2.3	- 210	-0.509	- 222	-0.425	+0.5	0.9
ERROR OF THE COEFFICIENTS (STANDARD DEVIATION)									
	3.4	*0.0082*	*0.40*	*8.6*	*0.0195*	*4.1*	*0.0095*	*0.14*	
	3.4	*0.0082*	*0.40*	*8.6*	*0.0195*	*4.1*	*0.0095*	*0.14*	
	9.1	*0.0223*	*0.76*	*31.3*	*0.0774*	*11.2*	*0.0277*	*0.26*	
	33.8	*0.0815*	*0.84*	*34.4*	*0.0774*	*16.5*	*0.0386*	*0.29*	
CONVERSIONS									
A	*+ 6*	*-0.066*	*+ 0.1*	*+ 3*	*+0.004*	*+ 3*	*-0.021*	*+0.0*	
B	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	

Table 9

Retention indices and thermodynamic data for 152 solutes in C78/PCN mixtures where data for an ideal solvent with X = PCN, idPCN, are also given. For symbols and explanations see Table 8.

No.	*Compound*	*Temp. range*	*n*	*Retention index : C78 / PCN*						
				PCN- C78		*Mixture*		*id([CN] =1) - C78*		*σ*
				ΔI_{130}	$10 \times \Delta A_T$	A_L	$10 \times A_{LT}$	$\Delta' I_{130}$	$10 \times \Delta' A_T$	
		(°C)			*(K^{-1})*		*(K^{-1})*	*(l mol^{-1})*	*(K^{-1}l mol^{-1})*	
HYDROCARBONS										
n-Alkanes										
00.05	Pentane	90-210	21							
00.06	Hexane	90-210	21							
00.07	Heptane	90-210	21							
00.08	Octane	90-210	21							
00.09	Nonane	90-210	21							
00.10	Decane	90-210	21							
00.11	Undecane	150-210	12							
00.12	Dodecane	150-210	12							
00.13	Tridecane	150-210	12							
00.14	Tetradecane	150-210	12							
Isoalkanes										
10.01	2,2-Dimethylbutane	90-170	15	- 0.0**	-0.09**	+ 0.6	+0.04	+ 0.9	-0.06	0.33
10.02	2,3-Dimethylbutane	90-170	15	- 0.0	-0.14*	- 0.2**	-0.08**	- 0.3	-0.32	0.37
10.03	2,2-Dimethylpentane	90-170	15	- 0.1**	-0.19	- 0.3**	-0.33*	- 0.6	-0.75	0.29
10.04	2,3-Dimethylpentane	90-170	15	+ 0.1**	-0.11^{s}	+ 0.0**	+0.10**	+ 0.1	-0.01	0.23
10.05	2,4-Dimethylpentane	90-170	15	- 0.7	-0.12	+ 0.4**	-0.23	- 0.5	-0.51	0.44
10.06	2,2-Dimethylhexane	90-170	15	- 0.3^{s}	-0.23	- 0.4**	-0.25*	- 1.1	-0.70	0.22
10.07	2,3-Dimethylhexane	90-170	15	+ 0.4	+0.03**	- 0.0**	+0.26	+ 0.6	+0.42	0.11
10.08	2,4-Dimethylhexane	90-170	15	- 0.3^{s}	-0.01**	- 0.5**	+0.07**	- 1.1	+0.08	0.26
10.09	3,4-Dimethylhexane	90-170	15	+ 0.6	+0.06*	- 1.5	+0.25^{s}	- 1.3	+0.43	0.17
10.10	2,2,3-Trimethylbutane	90-170	15	+ 0.4^{s}	+0.34	- 0.7**	+0.77	- 0.3	+1.59	0.27
10.11	2,2,4-Trimethylpentane	90-170	15	- 0.7	+0.12^{s}	- 0.6**	+0.39^{s}	- 1.8	+0.71	0.25
10.12	2,3,4-Trimethylpentane	90-170	15	+ 0.6	+0.26	- 1.2	+0.54	- 0.8	+1.14	0.18
1-Alkenes										
11.05	1-Pentene	90-170	15	+ 4.0	-0.44	- 0.6**	-0.93	+ 4.7	-1.92	0.76
11.06	1-Hexene	90-170	15	+ 4.0	-0.55	+ 1.0*	+0.11**	+ 7.1	-0.56	0.28
11.07	1-Heptene	90-170	15	+ 4.8	-0.29	+ 1.5*	+0.19**	+ 9.0	-0.06	0.37
11.08	1-Octene	90-170	15	+ 4.7	-0.19*	+ 0.4**	+0.41**	+ 7.3	+0.38	0.58
11.09	1-Nonene	90-170	15	+ 5.0	-0.06**	+ 0.5**	+0.43**	+ 7.9	+0.60	0.67
11.10	1-Decene	90-170	15	+ 4.6	+0.20**	- 0.2**	+0.78**	+ 6.4	+1.46	0.86

No.	Thermodynamic data : C78 / PCN								
	PCN - C78			Mixture		id([CN] =1) - C78			σ
	ΔH (cal mol^{-1})	ΔS (cal mol^{-1}K^{-1})	ΔC$_P$ (cal mol^{-1}K^{-1})	h (cal mol^{-1})	s (cal mol^{-1} K^{-1})	ΔH' (cal l mol^{-2})	ΔS' (cal l mol^{-2}K^{-1})	ΔC$_P$' (cal l mol^{-2}K^{-1})	(cal mol^{-1})
HYDROCARBONS									
n-Alkanes									
00.05	+ 114	+0.012	-3.2	-194	-0.627	- 189	-1.058	- 5.1	5.6
00.06	+ 101	-0.029	-3.0	-193	-0.627	- 208	-1.121	- 4.9	4.8
00.07	+ 88	-0.069	-2.9	-192	-0.627	- 227	-1.182	- 4.8	4.7
00.08	+ 74	-0.110	-2.7	-190	-0.627	- 246	-1.245	- 4.5	4.2
00.09	+ 61	-0.150	-2.6	-189	-0.627	- 265	-1.306	- 4.4	3.2
00.10	+ 48	-0.191	-2.4	-188	-0.627	- 283	-1.368	- 4.2	3.6
00.11	+ 35	-0.231	-2.2	-187	-0.627	- 302	-1.429	- 3.9	4.7
00.12	+ 21	-0.272	-2.1	-185	-0.627	- 321	-1.492	- 3.8	4.3
00.13	+ 8	-0.312	-1.9	-184	-0.627	- 339	-1.553	- 3.6	5.4
00.14	- 5	-0.353	-1.8	-183	-0.627	- 358	-1.616	- 3.5	6.3
Isoalkanes									
10.01	+ 87	-0.057**	-3.2^{s}	-191	-0.612	- 222	-1.133	- 5.2	2.1
10.02	+ 70	-0.099	-5.2	-211	-0.673	- 278	-1.287	- 8.1	1.7
10.03	+ 58	-0.138	-2.9^{s}	-261	-0.798	- 365	-1.521	- 5.0	1.7
10.04	+ 65	-0.123	-1.8^{s}	-172	-0.576	- 229	-1.183	- 3.2	1.1
10.05	+ 76	-0.093	-6.3	-248	-0.758	- 323	-1.402	- 9.7	0.8
10.06	+ 40	-0.191	-3.1	-242	-0.758	- 368	-1.545	-5.3	1.2
10.07	+ 80	-0.088	-2.7	-135	-0.489	- 157	-1.015	- 4.4	0.6
10.08	+ 84	-0.082	-4.4	-174	-0.592	- 211	-1.158	- 6.9	1.2
10.09	+ 81	-0.085	-2.9	-121	-0.474	- 140	-0.997	- 4.7	0.9
10.10	+ 160	+0.118	-2.7	- 21**	-0.214^{s}	+ 117	-0.333	- 3.9	1.5
10.11	+ 120	-0.001**	-2.3^{s}	-102^{s}	-0.413	- 58	-0.789	- 3.7	1.4
10.12	+ 125	+0.027	-3.8	- 67	-0.335	- 0	-0.640	- 5.7	0.9
1-Alkenes									
11.05	- 24**	-0.270	-4.5**	-393	-1.125	- 658	-2.142	- 7.7	4.1
11.06	- 62	-0.373	-4.4	-178	-0.576	- 406	-1.506	- 7.1	1.0
11.07	- 23^{s}	-0.273	-4.7	-165	-0.541	- 331	-1.314	- 7.4	1.2
11.08	- 13**	-0.258	-5.3	-103*	-0.407	- 235	-1.116	- 8.1	2.2
11.09	- 2**	-0.237	-4.7^{s}	- 98**	-0.396*	- 213	-1.073	- 7.3	3.2
11.10	+ 42**	-0.144**	-4.1**	- 15**	-0.202**	- 38	-0.677	- 6.2	4.6

(Continued on pages 412 and 413)

Table 9 (*continued*)

No.	Compound	Temp. range	n	Retention index : C78 / PCN						
				PCN- C78		Mixture		id([CN] =1) - C78		σ
		(°C)		ΔI_{130}	10 × ΔA_T (K^{-1})	A_L	10 × A_{LT} (K^{-1})	ΔI_{130} ($l\ mol^{-1}$)	10 × ΔA_T ($K^{-1} l\ mol^{-1}$)	
1-Alkynes										
12.05	1-Pentyne	90-170	15	+19.1	-0.34	+ 6.0	+1.43	+ 36.1	+1.89	0.62
12.06	1-Hexyne	90-170	15	+19.9	-0.39	+ 6.2	+0.48**	+ 37.4	+0.47	0.57
12.07	1-Heptyne	90-170	15	+20.6	-0.16**	+ 8.6	-0.13**	+ 41.8	-0.03	0.75
12.08	1-Octyne	90-170	15	+20.5	-0.19^{s}	+ 5.6	+0.21**	+ 37.4	+0.37	0.42
12.09	1-Nonyne	90-170	15	+20.6	-0.08**	+ 6.6	-0.04**	+ 38.9	+0.18	0.52
12.10	1-Decyne	90-170	15	+20.8	+0.03**	+ 6.8	+0.00**	+ 39.5	+0.40	0.59
Alkynes										
13.01	2-Hexyne	90-170	15	+16.1	-0.47^{s}	+ 1.6**	+0.55	+ 25.4	+0.35	0.97
13.02	3-Hexyne	90-170	15	+14.0	-0.07**	+ 3.9	-0.03**	+ 25.6	+0.09	0.56
13.03	4-Octyne	90-170	15	+12.9	-0.02**	+ 3.2	-0.03**	+ 23.1	+0.14	0.50
Monocyclic hydrocarbons										
14.05	Cyclopentane	90-170	15	+ 2.1	-0.33	- 1.5	-0.17**	+ 0.8	-0.71	0.17
14.06	Cyclohexane	90-170	15	+ 1.7	+0.05**	- 2.7	+0.45	- 1.4	+0.70	0.22
14.07	Cycloheptane	90-170	15	+ 2.4	+0.34	- 3.1	+0.37	- 0.9	+1.01	0.31
14.08	Cyclooctane	90-170	15	+ 3.0	+0.57	- 4.8	+0.99	- 2.4	+2.21	0.27
14.10	Cyclodecane	130-210	15	+ 4.9	+0.25	- 4.4	+0.36	+ 0.8	+0.88	0.38
Bicyclic hydrocarbons										
15.01	*cis*-Hydrindane	130-210	15	+ 3.3	+0.30	- 2.4	-0.32^{s}	+ 1.3	-0.02	0.20
15.02	*trans*-Hydrindane	130-210	15	+ 1.6	+0.56	- 0.8**	-0.11**	+ 1.2	+0.66	0.52
15.03	*cis*-Decalin	130-210	15	+ 4.4	+0.47	+ 2.0**	-0.43**	+ 9.2	+0.14	0.42
15.04	*trans*-Decalin	130-210	15	+ 2.7	+0.27	- 3.4	-0.22**	- 1.0	+0.06	0.27
Methylcyclohexanes (MCH)										
16.01	Methylcyclohexane	90-170	15	+ 1.1	+0.09**	- 2.8	-0.03**	- 2.4	+0.06	0.31
16.02	*cis*-1,2-Di MCH	90-170	15	+ 2.3	+0.16*	- 1.4*	+0.21**	+ 1.3	+0.54	0.40
16.03	*trans*-1,2-Di MCH	90-170	15	+ 1.6	+0.17^{s}	- 1.9	+0.39*	- 0.4	+0.79	0.36
16.04	*cis*-1,4-Di MCH	90-170	15	+ 2.0	+0.16	- 1.3	-0.16**	+ 1.0	+0.01	0.19
16.05	*trans*-1,4-Di MCH	90-170	15	+ 1.4	+0.17	- 1.5	+0.15*	- 0.1	+0.46	0.16
Cyclohexenes										
17.01	Cyclohexene	90-170	15	+ 6.9	+0.11*	- 1.4^{s}	+0.00**	+ 7.9	+0.23	0.33
17.02	1,3-Cyclohexadiene	90-170	15	+14.5	+0.33	+ 1.4**	+1.23	+ 22.9	+2.44	0.56
17.03	1,4-Cyclohexadiene	90-170	15	+14.7	+0.51	+ 4.2	+0.76	+ 27.2	+2.07	0.25

No.	Thermodynamic data : C78 / PCN								
	PCN - C78			Mixture		id([CN] =1) - C78			σ
	ΔH (cal mol^{-1})	ΔS (cal mol^{-1}K^{-1})	ΔC_P (cal mol^{-1}K^{-1})	h (cal mol^{-1})	s (cal mol^{-1} K^{-1})	$\Delta H'$ (cal l mol^{-2})	$\Delta S'$ (cal l mol^{-2}K^{-1})	$\Delta C_P'$ (cal l mol^{-2}K^{-1})	(cal mol^{-1})
1-Alkynes									
12.05	- 156	-0.383	-6.3	+ 68**	+0.106**	- 139	-0.430	- 9.2	2.8
12.06	- 185	-0.464	-3.9*	-160*	-0.445*	- 500	-1.318	- 6.3	3.3
12.07	- 155	-0.401	-3.6**	-320^{s}	-0.828	- 684	-1.770	- 6.2	4.3
12.08	- 172	-0.459	-2.5	-203	-0.583	- 553	-1.529	- 4.5	2.4
12.09	- 165	-0.452	-1.9**	-269	-0.739	- 637	-1.741	- 3.7	3.0
12.10	- 159	-0.442	-2.7**	-261	-0.721	- 618	-1.706	- 4.9	3.3
Alkynes									
13.01	- 163	-0.493	+4.6**	- 79**	-0.324**	- 377	-1.245	+ 5.7	4.5
13.02	- 62	-0.244	-5.7	-234	-0.678	- 456	-1.399	- 8.9	1.8
13.03	- 65	-0.287	-5.4	-225	-0.672	- 458	-1.472	- 8.5	1.2
Monocyclic hydrocarbons									
14.05	+ 6**	-0.236	-2.1	-219	-0.711	- 377	-1.528	- 3.9	0.8
14.06	+ 76	-0.074	-3.3	- 70*	-0.359	- 72	-0.815	- 5.1	1.3
14.07	+ 107	+0.004**	-5.1	- 84	-0.403	- 52	-0.773	- 7.7	1.0
14.08	+ 129	+0.055^{s}	-4.7	+ 59*	-0.077**	+ 176	-0.252	- 6.8	1.2
14.10	+ 41**	-0.162**	-3.1	- 82	-0.424	- 146	-1.047	- 4.9	1.5
Bicyclic hydrocarbons									
15.01	+ 83	-0.066**	-3.1	-221	-0.739	- 279	-1.349	- 5.2	0.9
15.02	+ 209	+0.223**	-4.7^{s}	-199^{s}	-0.666	- 73	-0.839	- 7.1	2.5
15.03	+ 92**	-0.041**	-3.4*	-283	-0.842	- 346	-1.435	- 5.7	2.1
15.04	+ 92^{s}	-0.059**	-3.6	-192	-0.684	- 232	-1.274	- 5.8	1.2
Methylcyclohexanes (MCH)									
16.01	+ 81	-0.072*	-4.4	-172	-0.615	- 214	-1.182	- 6.9	1.6
16.02	+ 71	-0.099	-0.7	-136	-0.513	- 173	-1.064	- 1.6	1.1
16.03	+ 85	-0.072	-0.6**	- 92	-0.409	- 92	-0.885	- 1.4	0.7
16.04	+ 77	-0.079	-3.5	-211	-0.696	- 271	-1.297	- 5.7	1.2
16.05	+ 88	-0.059	-2.7	-145	-0.533	- 162	-1.041	- 4.4	1.0
Cyclohexenes									
17.01	+ 33^{s}	-0.115	-4.3	-179	-0.613	- 275	-1.198	- 6.8	1.7
17.02	- 1**	-0.104*	-1.9**	+ 50**	-0.011**	+ 27	-0.269	- 2.8	2.6
17.03	+ 37	-0.007**	-4.2	- 79*	-0.294	- 97	-0.520	- 6.2	1.4

(Continued on pages 414 and 415)

Table 9 (continued)

No.	Compound	Temp. range (°C)	n	Retention index : C78 / PCN						
				PCN- C78		Mixture		id([CN] =1) - C78		σ
				ΔI_{130}	10 x ΔA_T (K^{-1})	A_L	10 x A_{LT} (K^{-1})	$\Delta I'_{130}$ (l mol^{-1})	10 x $\Delta A'_T$ ($K^{-1} l$ mol^{-1})	
Alkylbenzenes										
18.00	Benzene	90-170	15	+24.6	+0.38	+ 2.0	+0.79	+ 38.2	+2.02	0.35
18.01	Toluene	90-170	15	+24.4	+0.41	+ 3.1	+0.24*	+ 39.5	+1.29	0.18
18.02	Ethylbenzene	90-170	15	+23.8	+0.51	+ 3.6	+0.05**	+ 39.3	+1.16	0.33
Miscellaneous										
19.01	Adamantane	130-210	15	+ 3.7	+0.93	- 1.2**	+0.38**	+ 3.7	+1.91	0.58
19.02	Naphthalene	130-210	15	+42.9	+0.60	+ 9.4	-0.50**	+ 74.9	+0.82	0.78
19.03	Azulene	130-210	15	+54.6	+1.06	+18.3	+1.42**	+104.7	+4.51	1.48
ALKANE DERIVATIVES										
1-Fluoroalkanes										
20.05	1-Fluoropentane	90-170	15	+25.3	-0.07**	+ 6.9	-0.36**	+ 46.1	-0.19	0.44
20.06	1-Fluorohexane	90-170	15	+25.7	-0.03**	+ 7.2	-0.31**	+ 47.1	-0.06	0.37
20.07	1-Fluoroheptane	90-170	15	+26.1	+0.05**	+ 7.7	-0.21**	+ 48.4	+0.21	0.33
20.08	1-Fluorooctane	90-170	15	+26.6	+0.03**	+ 8.6	-0.36^{s}	+ 50.4	-0.01	0.24
1,1,1-Trifluoroalkanes										
21.08	1,1,1-Trifluorooctane	90-170	15	+26.2	+0.03**	+11.1	-0.13**	+ 53.4	+0.35	0.26
21.10	1,1,1-Trifluorodecane	90-170	15	+26.6	-0.25	+11.4	-0.55	+ 54.4	-0.65	0.23
1-Chloroalkanes										
22.04	1-Chlorobutane	90-170	15	+27.0	+0.08**	+ 6.2	-0.60*	+ 47.5	-0.31	0.39
22.05	1-Chloropentane	90-170	15	+26.9	+0.42	+ 6.2	+0.63	+ 47.5	+1.94	0.33
22.06	1-Chlorohexane	90-170	15	+27.1	+0.35	+ 5.9	+0.46	+ 47.4	+1.59	0.51
1-Bromoalkanes										
23.03	1-Bromopropane	90-170	15	+28.3	+0.22*	+ 6.4	+0.15**	+ 49.8	+0.98	0.54
23.04	1-Bromobutane	90-170	15	+27.9	+0.25^{s}	+ 5.4	+0.36**	+ 47.8	+1.31	0.53
23.05	1-Bromopentane	90-170	15	+28.0	+0.36	+ 5.0	+0.46**	+ 47.4	+1.61	0.61
1-Cyanoalkanes										
24.02	Cyanoethane	90-170	15	+89.6	-0.19**	+39.0	-1.89^{s}	+184.0	-1.29	1.33
24.03	1-Cyanopropane	90-170	15	+88.5	-0.35	+32.6	-1.12	+173.4	-0.52	0.34
24.04	1-Cyanobutane	90-170	15	+88.9	-0.23	+32.2	-0.69^{s}	+173.4	+0.27	0.38
24.05	1-Cyanopentane	90-170	15	+89.7	-0.05**	+33.1	-0.54*	+175.9	+0.76	0.48

No.	Thermodynamic data : C78 / PCN								
	PCN - C78			Mixture		id([CN] =1) - C78			σ
	ΔH (cal mol^{-1})	ΔS (cal mol^{-1}K^{-1})	ΔC_P (cal mol^{-1}K^{-1})	h (cal mol^{-1})	s (cal mol^{-1} K^{-1})	$\Delta H'$ (cal l mol^{-2})	$\Delta S'$ (cal l mol^{-2}K^{-1})	$\Delta C_P'$ (cal l mol^{-2}K^{-1})	(cal mol^{-1})
Alkylbenzenes									
18.00	- 92	-0.195	-2.6*	- 31**	-0.200**	- 191	-0.604	- 4.0	1.9
18.01	- 99	-0.227	-3.5	-171	-0.536	- 401	-1.128	- 5.6	0.9
18.02	- 84	-0.205	-4.7	-215	-0.644	- 447	-1.257	- 7.4	1.7
Miscellaneous									
19.01	+ 234	+0.303**	-4.9^{s}	-121**	-0.477^{s}	+ 77	-0.454	- 7.2	2.8
19.02	- 179*	-0.249**	-5.4*	-365	-0.955	- 750	-1.652	- 8.7	3.7
19.03	- 724	-1.436	+7.2	-129**	-0.259**	-1 129	-2.204	+ 8.8	3.2
ALKANE DERIVATIVES									
1-Fluoroalkanes									
20.05	- 167	-0.335	-5.3	-343	-0.899	- 721	-1.744	- 8.6	2.1
20.06	- 178	-0.386	-4.3	-331	-0.874	- 723	-1.792	- 7.2	1.7
20.07	- 177	-0.393	-4.2	-310	-0.820	- 694	-1.729	- 6.9	1.5
20.08	- 202	-0.461	-3.4	-350	-0.914	- 785	-1.957	- 6.0	1.2
1,1,1-Trifluroalkanes									
21.08	- 174	-0.383	-3.3	-326	-0.817	- 704	-1.689	- 5.7	1.4
21.10	- 260	-0.617	-1.3**	-414	-1.039	- 953	-2.342	- 3.3	1.3
1-Chloroalkanes									
22.04	- 166	-0.346	-1.5**	-378	-1.003	- 771	-1.914	-3.3	2.3
22.05	- 107	-0.211	-2.8^{s}	-112^{s}	-0.352	- 316	-0.811	-4.5	1.8
22.06	- 140	-0.303	-3.2*	-143*	-0.437^{s}	- 410	-1.070	-5.2	2.7
1-Bromoalkanes									
23.03	- 150	-0.287	-2.7**	-216	-0.600	- 517	-1.252	- 4.6	2.9
23.04	- 152	-0.306	-4.6	-160^{s}	-0.480	- 448	-1.127	- 7.2	2.2
23.05	- 149	-0.309	-4.6^{s}	-136*	-0.431^{s}	- 413	-1.071	- 7.2	2.9
1-Cyanoalkanes									
24.02	- 839	-1.102	-6.7*	-988	-2.045	-2 349	-3.867	-11.9	4.9
24.03	- 895	-1.340	-1.4*	-776	-1.619	-2 159	-3.678	- 4.3	1.2
24.04	- 868	-1.303	-1.8	-656	-1.358	-1 963	-3.284	- 4.6	1.9
24.05	- 861	-1.302	-1.4**	-632	-1.297	-1 922	-3.203	- 4.0	2.8

(Continued on pages 416 and 417)

Table 9 (*continued*)

No.	Compound	Temp. range (°C)	n	Retention index : C78 / PCN						σ
				PCN- C78		Mixture		id([CN] =1) - C78		
				ΔI_{130}	10 × ΔA_T (K^{-1})	A_L	10 × A_{LT} (K^{-1})	ΔI_{130} ($l\ mol^{-1}$)	10 × ΔA_T ($K^{-1} l\ mol^{-1}$)	
1-Nitroalkanes										
25.02	Nitroethane	90-170	15	+90.2	-1.19	+32.2	-0.57**	+175.2	-0.91	0.89
25.03	1-Nitropropane	90-170	15	+86.2	-0.86	+30.0	-0.11**	+166.4	+0.13	0.44
25.04	1-Nitrobutane	90-170	15	+85.2	-0.69	+29.9	-0.36^{s}	+164.8	+0.00	0.25
25.05	1-Nitropentane	90-170	15	+84.4	-0.55	+30.6	-0.30**	+164.7	+0.29	0.29
1-Acetoxyalkanes										
26.03	1-Acetoxypropane	90-170	15	+41.2	-0.21*	+12.4	-0.57**	+ 76.7	-0.42	0.59
26.04	1-Acetoxybutane	90-170	15	+41.7	-0.20**	+12.8	-0.64**	+ 77.9	-0.49	0.69
26.05	1-Acetoxypentane	90-170	15	+42.1	-0.28*	+12.4	-0.58**	+ 77.9	-0.52	0.71
1-Alkanols										
27.04	1-Butanol	90-170	15	+64.8	-2.37	+27.6	-1.16**	+132.0	-3.85	1.11
27.05	1-Pentanol	90-170	15	+66.5	-2.18	+28.4	-0.99	+135.6	-3.29	1.13
27.06	1-Hexanol	90-170	15	+67.5	-2.23	+30.0	-1.54*	+139.3	-4.13	1.22
27.07	1-Heptanol	90-170	15	+67.6	-1.84	+32.6	-2.02	+143.2	-4.22	1.06
2-Alkanols										
28.04	2-Butanol	90-170	15	+54.3	-1.49	+19.5	-0.85^{s}	+105.5	-2.39	0.55
28.05	2-Pentanol	90-170	15	+55.3	-1.38	+19.9	-0.07**	+107.6	-1.09	0.36
28.06	2-Hexanol	90-170	15	+56.3	-1.41	+21.2	-0.37**	+110.9	-1.54	0.38
28.07	2-Heptanol	90-170	15	+56.9	-1.39	+22.7	-0.66^{s}	+113.8	-1.89	0.45
2-Methyl-2-alkanols										
29.04	2-Methyl-2-propanol	90-170	15	+49.8	-1.88	+12.5	-0.51**	+ 89.0	-2.61	0.52
29.05	2-Methyl-2-butanol	90-170	15	+49.2	-1.68	+15.2	-0.65*	+ 92.0	-2.49	0.52
29.06	2-Methyl-2-pentanol	90-170	15	+49.3	-1.42	+16.4	-0.76^{s}	+ 93.9	-2.26	0.43
29.07	2-Methyl-2-hexanol	90-170	15	+49.6	-1.32	+16.9	-1.22	+ 95.0	-2.77	0.41
1-Alkanethiols										
30.04	1-Butanethiol	90-170	15	+25.6	-1.01	+ 5.5	-0.56**	+ 44.4	-1.84	0.76
30.05	1-Pentanethiol	90-170	15	+26.3	-0.82	+ 5.2	-0.74	+ 44.9	-1.82	0.86
30.06	1-Hexanethiol	90-170	15	+26.5	-0.83	+ 4.5	-0.24	+ 44.3	-1.13	0.89
2-Alkanones										
31.04	2-Butanone	90-170	15	+56.7	-0.83	+17.8	-1.46	+106.5	-2.31	0.89
31.05	2-Pentanone	90-170	15	+56.1	-0.55	+17.9	-0.92^{s}	+105.9	-1.14	0.56

No.	Thermodynamic data : C78 / PCN								σ
	PCN - C78			Mixture		id([CN] = 1) - C78			
	ΔH (cal mol^{-1})	ΔS (cal $mol^{-1} K^{-1}$)	ΔC_p (cal $mol^{-1} K^{-1}$)	$\bar{h}$ (cal mol^{-1})	s (cal $mol^{-1} K^{-1}$)	$\Delta' H$ (cal l mol^{-2})	$\Delta' S$ (cal l $mol^{-2} K^{-1}$)	$\Delta' C_p$ (cal l $mol^{-2} K^{-1}$)	(cal mol^{-1})
1-Nitroalkanes									
25.02	-1 089	-1.771	-4.5*	-659	-1.301	-2 257	-3.809	- 2.8	3.5
25.03	- 974	-1.588	-2.6§	-532	-1.063	-1 944	-3.287	- 5.8	1.6
25.04	- 941	-1.547	-0.9**	-561	-1.151	-1 947	-3.766	- 3.4	1.4
25.05	- 926	-1.528	+0.2**	-564	-1.159	-1 932	-3.367	- 1.8	1.5
1-Acetoxyalkanes									
26.03	- 366	-0.666	+2.2**	-437	-1.066	-1 090	-2.337	+ 1.7	2.2
26.04	- 378	-0.705	+2.1**	-451	-1.104	-1 129	-2.452	+ 1.4	2.5
26.05	- 417	-0.813	+3.1*	-431	-1.065	-1 159	-2.557	+ 2.8	2.4
1-Alkanols									
27.04	-1 070	-2.102	+5.6*	-743	-1.616	-2 427	-4.917	+ 4.8	5.4
27.05	-1 037	-2.024	+6.1§	-694	-1.500	-2 311	-4.647	+ 5.7	4.2
27.06	-1 073	-2.123	+7.7	-820	-1.802	-2 540	-5.211	+ 7.6	4.1
27.07	-1 003	-1.953	+3.8**	-944	-2.081	-2 615	-5.361	+ 2.0	4.7
2-Alkanols									
28.04	- 769	-1.434	-1.1**	-593	-1.340	-1 824	-3.668	- 3.8	3.5
28.05	- 761	-1.456	+0.8**	-411	-0.905	-1 563	-3.106	- 0.8	2.0
28.06	- 780	-1.508	+0.1**	-479	-1.064	-1 686	-3.404	- 1.9	2.2
28.07	- 801	-1.571	+1.1**	-556	-1.245	-1 825	-3.747	- 0.8	2.3
2-Methyl-2-alkanols									
29.04	- 805	-1.586	+2.2**	-428	-1.029	-1 667	-3.507	+ 0.9	2.9
29.05	- 767	-1.550	+3.6	-504	-1.190	-1 725	-3.696	+ 2.8	1.9
29.06	- 709	-1.421	+1.8*	-524	-1.231	-1 674	-3.576	+ 0.3	1.5
29.07	- 705	-1.418	+0.6**	-617	-1.462	-1 802	-3.905	- 1.6	1.9
1-Alkanethiols									
30.04	- 383	-0.924	+3.6*	-360	-0.971	-1 059	-2.701	+ 3.4	2.7
30.05	- 365	-0.886	+5.0	-392	-1.058	-1 080	-2.774	+ 5.4	1.9
30.06	- 380	-0.930	+5.4	-275	-0.781	- 938	-2.453	+ 6.1	2.6
2-Alkanones									
31.04	- 655	-1.109	-4.2**	-693	-1.612	-1 803	-3.591	- 8.2	4.8
31.05	- 598	-1.032	-3.5§	-563	-1.307	-1 551	-3.085	- 6.9	2.1

(Continued on pages 418 and 419)

Table 9 (*continued*)

No.	*Compound*	*Temp. range* (°C)	*n*	*Retention index : C78 / PCN*						*σ*
				PCN- C78		*Mixture*		*id([CN] =1) - C78*		
				ΔI_{130}	$10 \times \Delta A_T$ (K^{-1})	A_L	$10 \times A_{LT}$ (K^{-1})	$\Delta I'_{130}$ ($l\ mol^{-1}$)	$10 \times \Delta A'_T$ ($K^{-1} l\ mol^{-1}$)	
31.06	2-Hexanone	90-170	15	+57.1	-0.39	+17.9	-0.55*	+107.4	-0.36	0.47
31.07	2-Heptanone	90-170	15	+57.6	-0.28[s]	+18.5	-0.36**	+108.9	+0.08	0.60
Aldehydes										
32.05	Pentanal	90-170	15	+50.5	-0.68	+15.8	-1.42	+ 94.8	-2.14	0.42
32.06	Hexanal	90-170	15	+51.9	-0.48	+14.9	-0.74	+ 95.6	-0.87	0.27
32.07	Heptanal	90-170	15	+52.6	-0.29	+16.1	-0.71	+ 98.3	-0.53	0.19
Ethers										
33.06	Dipropylether	90-170	15	+12.9	-0.29	+ 3.8	+0.05**	+ 23.9	-0.13	0.12
33.08	Dibutylether	90-170	15	+12.6	-0.07*	+ 3.7	+0.11**	+ 23.4	+0.27	0.17
Halomethanes										
37.01	Dichloromethane	90-170	15	+42.8	+0.26[s]	+12.4	-0.21**	+ 79.1	+0.79	0.58
37.02	Trichloromethane	90-170	15	+40.3	-0.34	+11.9	-0.65*	+ 74.7	-0.74	0.48
37.03	Tetrachloromethane	90-170	15	+10.3	-0.07**	- 0.2**	-0.46*	+ 14.4	-0.63	0.41
37.04	CF_2Br_2	90-170	15	+14.8	-0.68[s]	- 0.9**	+0.91**	+ 19.9	+0.51	1.35
HALOBENZENES										
38.01	Fluorobenzene	90-170	15	+30.9	-0.03**	+ 6.2	+0.25**	+ 53.2	+0.80	0.28
38.02	Hexafluorobenzene	90-170	15	+31.1	-0.13**	+11.2	-0.24**	+ 60.6	+0.02	0.43
38.03	Trifluoromethylbenzene	90-170	15	+38.0	+0.14*	+11.4	+0.32**	+ 70.8	+1.31	0.37
38.04	Chlorobenzene	90-170	15	+32.6	+0.24*	+ 5.2	+0.65*	+ 54.3	+1.77	0.59
38.05	Bromobenzene	90-170	15	+35.0	+0.28*	+ 4.2	+0.88*	+ 56.3	+2.18	0.70
38.06	Iodobenzene	130-210	15	+36.9	+0.76	+ 4.4*	+0.52**	+ 59.3	+2.37	0.80
ALKYLPYRIDINES										
39.01	Pyridine	90-170	15	+53.7	-0.30[s]	+15.5	-0.29**	+ 99.1	+0.06	0.64
39.02	2-Picoline	90-170	15	+46.8	-0.30*	+13.2	-0.30**	+ 85.9	-0.07	0.88
39.03	3-Picoline	90-170	15	+57.1	-0.18**	+18.4	-0.17**	+108.1	+0.49	0.95
39.04	4-Picoline	90-170	15	+58.8	-0.39*	+19.2	-0.75**	+111.6	-0.61	1.04
39.05	2,3-Lutidine	130-210	15	+50.6	+0.04**	+13.2	+0.47**	+ 91.5	+1.57	0.68
39.06	2,4-Lutidine	130-210	15	+50.2	+0.07**	+14.8	+0.15**	+ 93.2	+1.17	0.79
39.07	2,5-Lutidine	130-210	15	+47.9	+0.26	+12.6	+0.34*	+ 86.7	+1.65	0.24
39.08	2,6-Lutidine	130-210	15	+40.5	-0.65	+12.4	-0.90[s]	+ 75.6	-1.53	0.62

No.	*Thermodynamic data : C78 / PCN*								
	PCN - C78			*Mixture*		*id([CN] =1) - C78*			*σ*
	ΔH (cal mol⁻¹)	*ΔS* (cal mol⁻¹K⁻¹)	*ΔCp* (cal mol⁻¹K⁻¹)	*h* (cal mol⁻¹)	*s* (cal mol⁻¹ K⁻¹)	*Δ'H* (cal l mol⁻²)	*Δ'S* (cal l mol⁻²K⁻¹)	*Δ'Cp* (cal l mol⁻²K⁻¹)	(cal mol⁻¹)
31.06	- 581	-0.994	-4.5	-478	-1.104	-1 410	-2.751	- 8.1	0.6
31.07	- 582	-1.009	-4.3	-442	-1.014	-1 363	-2.649	- 7.7	1.9
Aldehydes									
32.05	- 556	-0.959	-0.3**	-670	-1.584	-1 649	-3.386	- 2.5	2.4
32.06	- 542	-0.955	-1.8**	-500	-1.190	-1 400	-2.850	- 4.3	1.7
32.07	- 515	-0.897	-1.8*	-493	-1.164	-1 352	-2.732	- 4.2	1.2
Ethers									
33.06	- 100	-0.363	-2.1	-218	-0.642	- 490	-1.522	- 3.9	0.7
33.08	- 77	-0.327	-3.3	-202	-0.611	- 441	-1.442	- 5.5	0.5
Halomethanes									
37.01	- 268	-0.336	-6.1	-365	-0.877	- 838	-1.574	- 9.6	3.0
37.02	- 389	-0.720	-2.8**	-460	-1.129	-1 159	-2.513	- 5.5	2.9
37.03	- 35*	-0.239	-2.6*	-290	-0.869	- 516	-1.706	- 4.7	2.4
37.04	- 177	-0.526	+7.0**	+ 40**	-0.060**	- 233	-0.925	+ 9.3	7.1
HALOBENZENES									
38.01	- 236	-0.466	-3.4	-197	-0.556	- 606	-1.432	- 5.7	1.5
38.02	- 235	-0.424	-4.1	-352	-0.862	- 805	-1.755	- 6.9	1.9
38.03	- 269	-0.454	-3.6	-232	-0.575	- 674	-1.372	- 5.9	1.6
38.04	- 230	-0.455	-4.4*	- 96**	-0.328**	- 460	-1.106	- 6.9	3.0
38.05	- 257	-0.502	-4.4*	- 35**	-0.195**	- 413	-0.982	- 6.8	3.2
38.06	- 257*	-0.505*	-0.9**	-141**	-0.456**	- 560	-1.352	- 2.1	4.2
ALKYLPYRIDINES									
39.01	- 523	-0.908	+0.8**	-408	-0.961	-1 240	-2.455	- 0.4	2.8
39.02	- 471	-0.882	+2.3**	-389	-0.949	-1 163	-2.459	+ 1.7	4.2
39.03	- 557	-0.972	+2.5**	-404	-0.922	-1 274	-2.464	+ 1.9	4.7
39.04	- 616	-1.102	+4.9*	-537	-1.239	-1 538	-3.082	+ 5.0	2.9
39.05	- 589	-1.125	+1.6**	-246	-0.597	-1 119	-2.285	+ 0.8	2.2
39.06	- 570	-1.083	+1.3**	-303	-0.722	-1 172	-2.397	+ 0.3	3.7
39.07	- 425	-0.756	-1.0**	-250	-0.617	- 904	-1.815	- 2.5	1.1
39.08	- 602	-1.278	+1.5**	-458	-1.134	-1 462	-3.319	+ 0.1	2.4

(*Continued on pages 420 and 421*)

Table 9 (*continued*)

No.	Compound	Temp. range (°C)	*n*	Retention index : C78 / PCN PCN- C78 ΔI_{130}	 $10 \times \Delta A_T$ (K^{-1})	 Mixture A_L	 $10 \times A_{LT}$ (K^{-1})	 id([CN] =1) - C78 $\Delta I'_{130}$ ($l\ mol^{-1}$)	 $10 \times \Delta A'_T$ ($K^{-1} l\ mol^{-1}$)	 σ
39.09	3,4-Lutidine	130-210	15	+66.0	-0.66	+23.0	-1.01	+127.3	-1.23	0.49
39.10	3,5-Lutidine	130-210	15	+61.1	-0.58	+21.2	-1.05	+117.7	-1.26	0.51
39.11	2-Ethylpyridine	130-210	15	+42.9	-0.31	+10.9	-0.61*	+ 76.9	-0.61	0.47
39.12	3-Ethylpyridine	130-210	15	+53.1	-0.19^{s}	+11.2	-1.07	+ 91.9	-0.96	0.42
39.13	4-Ethylpyridine	130-210	15	+57.6	-0.25	+14.8	-0.16	+103.7	+0.36	0.65
39.14	2-Propylpyridine	130-210	15	+41.7	-0.73	+ 8.5	-0.34	+ 71.8	-0.88	0.39
39.15	4-Propylpyridine	130-210	15	+56.1	+0.53	+12.8	+1.31	+ 98.9	+3.54	0.67
39.16	2,3,6-Collidine	130-210	15	+40.4	-0.12*	+ 9.6	-0.47^{s}	+ 71.6	-0.19	0.31
39.17	2,4,6-Collidine	130-210	15	+41.7	-0.37	+11.0	-0.49	+ 75.4	-0.54	0.27
39.18	4-*tert*-Butylpyridine	130-210	15	+57.2	-0.48	+17.5	-0.99	+106.9	-1.13	0.37
39.19	3-Chloropyridine	90-170	15	+48.6	+0.02**	+10.0	-0.08**	+ 83.9	+0.68	0.46
ORGANOSILICON COMPOUNDS										
40.01	Tetramethylsilane	90-170	15	+ 2.6	+0.33^{s}	+ 6.7	-0.17**	+ 13.3	+0.35	0.71
40.02	Hexamethyldisilane	90-170	15	+ 1.6	+0.11*	+ 2.6	-0.40*	+ 5.9	-0.36	0.34
40.03	Hexamethyldisiloxane	90-170	15	+ 0.4**	-0.04**	+ 2.8	-0.64*	+ 4.5	-0.93	0.51
MISCELLANEOUS										
41.01	Carbon disulphide	90-170	15	+ 8.0	-0.81^{s}	- 3.3**	+0.61**	+ 6.7	-0.23	1.63
41.02	Tetramethyltin	90-170	15	+ 5.8	+0.38	- 0.3**	+1.08	+ 8.0	+2.16	0.31
41.03	Tetrahydrofuran	90-170	15	+32.3	-0.03**	+ 8.4	-0.28**	+ 58.3	+0.09**	0.38
41.04	1,4-Dioxane	90-170	15	+40.7	-0.12**	+ 8.4	-0.33**	+ 70.3	+0.00**	0.39
41.05	Thiophene	90-170	15	+27.8	+0.82	+ 4.3	+0.82	+ 46.2	+2.77	0.56
41.06	Cyclopentanone	90-170	15	+67.6	-0.23	+20.6	-0.91	+126.2	-0.48	0.41
41.07	Cyclohexanone	90-170	15	+68.4	+0.19**	+21.3	-0.59**	+128.5	+0.60	0.76
41.08	Cyclohexanol	90-170	15	+61.9	-1.76	+21.8	-1.29*	+119.6	-3.27	0.94
41.11	Nitrobenzene	130-210	15	+81.7	+0.35	+22.9	-0.35**	+149.9	+1.37	0.46
41.12	Benzyl alcohol	130-210	15	+99.4	-1.41	+36.2	-0.57**	+194.1	-1.06	0.95
41.13	2-Phenylethanol	130-210	15	+91.7	-1.06	+31.9	-0.69^{s}	+176.9	-0.89	0.42
41.14	Anisole	130-210	15	+42.9	+0.01**	+ 9.0	-0.11**	+ 74.3	+0.54	0.29
41.15	Phenetole	130-210	15	+40.1	+0.14*	+ 7.6	+0.56*	+ 68.4	+1.63	0.43
ERRORS:	*f (n-alkanes)*	*90-210*		*def.*						
	f (n-alkanes)	*150-210*		*def.*						
	f (solutes)	*90-170*		*0.65*	*0.22*	*2.19*	*0.77*	*3.28*	*1.13*	
	f (solutes)	*130-210*		*1.10*	*0.23*	*3.83*	*0.78*	*5.58*	*1.15*	
CONVERSION TO K_D:				*0*	*0*	*0*	*0*	*0*	*0*	

Table 9 (*continued*)

No.	*Thermodynamic data : C78 / PCN*								
	PCN - C78			*Mixture*		*id([CN] =1) - C78*			σ
	ΔH (cal mol^{-1})	ΔS (cal mol^{-1}K^{-1})	ΔC_P (cal mol^{-1}K^{-1})	h (cal mol^{-1})	s (cal mol^{-1} K^{-1})	$\Delta H'$ (cal l mol^{-2})	$\Delta S'$ (cal l mol^{-2}K^{-1})	$\Delta C_P'$ (cal l mol^{-2}K^{-1})	(cal mol^{-1})
39.09	- 882	-1.668	+3.1[s]	-571	-1.288	-1 942	-3.900	+ 1.9	1.9
39.10	- 778	-1.469	+1.8[**]	-579	-1.325	-1 820	-3.706	+ 0.2	2.1
39.11	- 527	-1.065	+0.4[**]	-400	-1.010	-1 273	-2.841	- 1.2	2.0
39.12	- 593	-1.109	+0.3[**]	-485	-1.220	-1 466	-3.149	- 1.5	2.1
39.13	- 732	-1.392	+2.5[*]	-376	-0.901	-1 488	-3.045	+ 1.6	1.8
39.14	- 462	-0.939	-2.3[s]	-332	-0.873	-1 099	-2.502	- 4.8	1.4
39.15	- 512	-0.880	+0.6[**]	- 38[**]	-0.096[**]	- 710	-1.213	+ 0.1	3.4
39.16	- 431	-0.876	-0.1[**]	-349	-0.906	-1 078	-2.458	- 1.7	1.5
39.17	- 532	-1.105	+1.1[**]	-372	-0.943	-1 245	-2.815	- 0.2	1.1
39.18	- 679	-1.290	-0.4[**]	-524	-1.242	-1 625	-3.390	- 2.7	1.9
39.19	- 517	-0.969	+0.1[**]	-305	-0.785	-1 114	-2.361	- 1.3	1.4
ORGANOSILICON COMPOUNDS									
40.01	+ 167	+0.195[s]	-7.7	-308	-0.813	- 253	-1.006	-11.5	3.7
40.02	+ 96	-0.026[**]	-3.3[s]	-310	-0.883	- 372	-1.459	- 5.5	2.0
40.03	+ 92	-0.045[**]	-2.9[**]	-363	-1.009	- 454	-1.665	- 5.1	2.8
MISCELLANEOUS									
41.01	- 162[s]	-0.595	+6.1[**]	- 25[**]	-0.255[**]	- 328	-1.362	+ 7.8	8.5
41.02	+ 122	+0.097	-3.3	+ 45[**]	-0.042[**]	+ 171	-0.085	- 4.6	1.8
41.03	- 242	-0.458	-3.9	-334	-0.864	- 800	-1.834	- 6.6	1.5
41.04	- 363	-0.654	-4.7	-336	-0.867	- 956	-2.070	- 7.9	1.6
41.05	- 41[*]	-0.022[**]	-5.9	- 71[**]	-0.270[**]	- 166	-0.431	- 8.5	2.9
41.06	- 662	-1.072	-1.2[**]	-569	-1.289	-1 622	-3.046	- 3.6	2.4
41.07	- 606	-0.947	+0.2[**]	-527	-1.185	-1 485	-2.725	- 1.4	3.9
41.08	- 931	-1.845	+6.1	-674	-1.545	-2 165	-4.533	+ 5.8	2.3
41.11	- 699	-1.038	-2.4[**]	-461	-1.013	-1 499	-2.549	- 5.0	2.4
41.12	-1 552	-2.904	+9.3	-619	-1.238	-2 848	-5.310	+ 9.8	1.0
41.13	-1 198	-2.146	+2.2[**]	-604	-1.257	-2 363	-4.352	+ 0.4	1.6
41.14	- 381	-0.714	-1.3[**]	-302	-0.791	- 936	-2.052	- 3.1	1.5
41.15	- 334	-0.643	+0.9[**]	-140	-0.411	- 649	-1.438	+ 0.4	1.9
E(contd)	*4.5*	*0.0091*	*0.38*	*7.8*	*0.0176*	*17.4*	*0.0378*	*0.54*	
	4.5	*0.0091*	*0.38*	*7.8*	*0.0176*	*17.4*	*0.0378*	*0.54*	
	9.1	*0.0224*	*0.76*	*31.4*	*0.0776*	*46.1*	*0.1131*	*1.07*	
	33.8	*0.0812*	*0.84*	*34.5*	*0.0776*	*68.3*	*0.1580*	*1.19*	
C(contd)	*- 0*	*-0.029*	*-0.0*	*- 1*	*-0.003*	*- 1*	*-0.045*	*- 0.1*	

Table 10
Retention indices and thermodynamic data for 152 solutes in C78/PSH mixtures where data for an ideal solvent with X = PSH, idPSH, are also given. For symbols and explanations see Table 8.

No.	Compound	Temp. range (°C)	n	Retention index : C78 / PSH						
				PSH-C78		Mixture		id([SH] = 1) - C78		σ
				ΔI_{130}	$10 \times \Delta A_T$ (K^{-1})	A_L	$10 \times A_{LT}$ (K^{-1})	$\Delta^{id} I_{130}$ ($l\ mol^{-1}$)	$10 \times \Delta^{id} A_T$ ($K^{-1} l\ mol^{-1}$)	
HYDROCARBONS										
n-Alkanes										
00.05	Pentane	90-210	21							
00.06	Hexane	90-210	21							
00.07	Heptane	90-210	21							
00.08	Octane	90-210	21							
00.09	Nonane	90-210	21							
00.10	Decane	90-210	21							
00.11	Undecane	150-210	12							
00.12	Dodecane	150-210	12							
00.13	Tridecane	150-210	12							
00.14	Tetradecane	150-210	12							
Isoalkanes										
10.01	2,2-Dimethylbutane	90-170	15	- 1.5	-0.28^{s}	+ 2.4	+1.00	+ 1.4	+1.09	0.29
10.02	2,3-Dimethylbutane	90-170	15	- 1.6	-0.34**	+ 3.2	+0.84*	+ 2.5	+0.77	0.63
10.03	2,2-Dimethylpentane	90-170	15	- 1.2	-0.37	+ 0.9	+0.36	- 0.5	-0.02	0.09
10.04	2,3-Dimethylpentane	90-170	15	- 0.4	-0.04**	+ 0.8^{s}	+0.08**	+ 0.6	+0.07	0.19
10.05	2,4-Dimethylpentane	90-170	15	- 1.2	-0.66	+ 1.8^{s}	+0.62*	+ 0.9	-0.05	0.41
10.06	2,2-Dimethylhexane	90-170	15	- 1.1	-0.22	+ 0.2**	+0.12**	- 1.4	-0.16	0.11
10.07	2,3-Dimethylhexane	90-170	15	- 0.3*	-0.19	+ 0.8**	+0.32**	+ 0.8	+0.20	0.30
10.08	2,4-Dimethylhexane	90-170	15	- 1.2	-0.09	+ 0.2**	+0.36	- 1.5	+0.39	0.21
10.09	3,4-Dimethylhexane	90-170	15	+ 0.0**	+0.17^{s}	- 0.6**	-0.04**	- 0.9	+0.19	0.19
10.10	2,2,3-Trimethylbutane	90-170	15	- 1.2	+0.66	+ 0.1**	+0.18**	- 1.6	+1.25	0.32
10.11	2,2,4-Trimethylpentane	90-170	15	- 1.5	+0.20	- 0.4**	+0.10**	- 2.8	+0.43	0.20
10.12	2,3,4-Trimethylpentane	90-170	15	- 0.1**	+0.20*	+ 0.1**	+0.44*	+ 0.1	+0.96	0.28
1-Alkenes										
11.05	1-Pentene	90-170	15	+ 1.1	-1.56	+ 1.7*	-0.44**	+ 3.9	-2.97	0.45
11.06	1-Hexene	90-170	15	+ 2.2	-1.05	+ 1.4*	-0.82^{s}	+ 5.2	-2.76	0.45
11.07	1-Heptene	90-170	15	+ 2.6	-0.78	+ 3.2	-0.38	+ 8.6	-1.66	0.15
11.08	1-Octene	90-170	15	+ 2.2	-0.53	+ 1.8	-0.84	+ 5.9	-2.01	0.16
11.09	1-Nonene	90-170	15	+ 2.7	-0.24	+ 0.7**	-0.64^{s}	+ 5.0	-1.28	0.35
11.10	1-Decene	90-170	15	+ 2.4	-0.21^{s}	+ 0.4**	-0.46^{s}	+ 4.1	-0.97	0.25

No.	*Thermodynamic data : C78 / PSH*								
	PSH - C78			*Mixture*		*id([SH] =1) - C78*			*σ*
	ΔH	*ΔS*	*ΔC$_P$*	*h̄*	*s*	*ΔH′*	*ΔS′*	*ΔC$_P$′*	
	(cal mol^{-1})	*(cal mol^{-1}K^{-1})*		*(cal mol^{-1})*	*(cal mol^{-1} K^{-1})*	*(cal l mol^{-2})*	*(cal l mol^{-2}K^{-1})*		*(cal mol^{-1})*
HYDROCARBONS									
n-Alkanes									
00.05	+ 80	-0.021	+0.6	+ 77	+0.073	+ 165	-0.070	+0.8	6.1
00.06	+ 89	-0.012	+0.4	+ 92	+0.073	+ 191	-0.081	+0.5	5.9
00.07	+ 99	-0.003	+0.1	+107	+0.073	+ 216	-0.090	+0.1	5.7
00.08	+109	+0.007	-0.2	+121	+0.073	+ 241	-0.097	-0.3	4.8
00.09	+119	+0.016	-0.5	+136	+0.073	+ 267	-0.108	-0.7	4.2
00.10	+129	+0.025	-0.7	+151	+0.073	+ 293	-0.119	-1.0	4.6
00.11	+138	+0.034	-1.0	+165	+0.073	+ 317	-0.127	-1.5	5.3
00.12	+148	+0.043	-1.3	+180	+0.073	+ 343	-0.138	-1.9	4.8
00.13	+158	+0.052	-1.6	+195	+0.073	+ 370	-0.148	-2.3	5.1
00.14	+168	+0.061	-1.9	+210	+0.073	+ 395	-0.159	-2.7	6.2
Isoalkanes									
10.01	+ 66	-0.084	+1.0**	+211	+0.421	+ 333	+0.329	+1.6	1.4
10.02	+ 66^{s}	-0.097**	+4.2*	+168*	+0.315	+ 272	+0.161	+6.1	3.2
10.03	+ 63	-0.097	+0.7*	+ 80	+0.046**	+ 133	-0.246	+0.9	0.6
10.04	+ 94	-0.017**	+0.4**	+ 97	+0.069**	+ 198	-0.107	+0.5	1.1
10.05	+ 34*	-0.171	+1.2**	+ 65**	+0.021**	+ 73	-0.381	+1.5	2.3
10.06	+ 87	-0.049	+0.0**	+ 82	+0.009**	+ 160	-0.255	-0.1	0.7
10.07	+ 87	-0.047**	+0.3**	+130	+0.118**	+ 227	-0.099	+0.4	1.6
10.08	+104	-0.012**	+0.4**	+163	+0.204^{s}	+ 298	+0.071	+0.6	1.2
10.09	+122	+0.042*	-0.1**	+147	+0.137*	+ 297	+0.044	-0.1	1.1
10.10	+174	+0.170	+1.3**	+269	+0.493	+ 554	+0.757	+2.3	1.5
10.11	+133	+0.060	+0.3**	+164	+0.212	+ 341	+0.187	+0.6	0.9
10.12	+126	+0.047	+1.6	+239	+0.378	+ 436	+0.399	+2.5	0.6
1-Alkenes									
11.05	-107	-0.469	+2.7**	-386	-1.042	- 749	-2.266	+2.6	2.5
11.06	- 50^{s}	-0.331	+3.4*	-342	-0.975	- 613	-1.993	+3.7	2.4
11.07	- 10*	-0.241	+1.3	-174	-0.574	- 323	-1.310	+1.1	0.7
11.08	+ 30	-0.159	+0.5**	-184	-0.652	- 293	-1.336	-0.0	0.9
11.09	+ 66	-0.082	+0.9	- 54	-0.383	- 69	-0.872	+0.8	1.7
11.10	+ 82	-0.061	+0.8**	+ 6	-0.275	+ 29	-0.715	+0.8	0.9

(Continued on pages 424 and 425)

Table 10 (*continued*)

No.	Compound	Temp. range (°C)	n	Retention index : C78 / PSH						σ
				PSH- C78		Mixture		id([SH] =1) - C78		
				ΔI_{130}	10 x ΔA_T (K^{-1})	A_L	10 x A_{LT} (K^{-1})	$\Delta I'_{130}$ ($l\ mol^{-1}$)	10 x $\Delta A'_T$ ($K^{-1} l\ mol^{-1}$)	
1-Alkynes										
12.05	1-Pentyne	90-170	15	+ 6.6	+0.09**	+ 2.2^{s}	-1.04	+13.1	-1.31	0.49
12.06	1-Hexyne	90-170	15	+ 7.2	-0.02**	+ 1.5	-0.92	+12.9	-1.29	0.22
12.07	1-Heptyne	90-170	15	+ 7.5	+0.19*	+ 2.3	-0.56^{s}	+14.7	-0.42	0.32
12.08	1-Octyne	90-170	15	+ 7.4	+0.31	+ 1.1*	-0.94	+12.7	-0.83	0.29
12.09	1-Nonyne	90-170	15	+ 7.5	+0.60	+ 0.1**	-0.84	+11.4	-0.26	0.35
12.10	1-Decyne	90-170	15	+ 7.4	+0.50	+ 1.9	-0.18**	+14.0	+0.61	0.31
Alkynes										
13.01	2-Hexyne	90-170	15	+ 6.2	-0.01**	+ 1.7	-0.12**	+11.9	-0.09	0.31
13.02	3-Hexyne	90-170	15	+ 5.7	-0.34^{s}	+ 1.4*	+0.46**	+10.7	+0.28	0.39
13.03	4-Octyne	90-170	15	+ 5.0	-0.14**	+ 0.2**	+0.34	+ 7.8	+0.37	0.42
Monocyclic hydrocarbons										
14.05	Cyclopentane	90-170	15	+ 2.7	-0.45*	- 0.2**	-0.10**	+ 3.7	-0.79	0.58
14.06	Cyclohexane	90-170	15	+ 2.6	-0.12**	+ 0.6**	+0.40^{s}	+ 4.8	+0.46	0.22
14.07	Cycloheptane	90-170	15	+ 3.9	+0.49	- 0.9**	-0.18**	+ 4.5	+0.51	0.31
14.08	Cyclooctane	90-170	15	+ 3.9	+1.26	- 0.7**	-0.56**	+ 4.9	+1.09	0.65
14.10	Cyclodecane	130-210	15	+ 4.4	+0.84	+ 0.2**	-0.02**	+ 7.0	+1.29	0.63
Bicyclic hydrocarbons										
15.01	*cis*-Hydrindane	130-210	15	+ 3.6	+0.68	- 1.2**	+0.19**	+ 3.7	+1.34	0.61
15.02	*trans*-Hydrindane	130-210	15	+ 1.2*	+0.94	- 4.1*	+0.56**	- 4.2	+2.22	0.60
15.03	*cis*-Decalin	130-210	15	+ 3.9	+1.09	- 0.8**	+0.50**	+ 4.8	+2.43	0.79
15.04	*trans*-Decalin	130-210	15	+ 2.8	+0.68	- 3.8*	+0.50**	- 1.4	+1.76	0.69
Methylcyclohexanes (MCH)										
16.01	Methylcyclohexane	90-170	15	+ 1.2	-0.18**	- 0.2**	+0.54*	+ 1.5	+0.56	0.42
16.02	*cis*-1,2-Di MCH	90-170	15	+ 2.8	-0.11**	+ 0.6**	+0.46**	+ 5.1	+0.57	0.49
16.03	*trans*-1,2-Di MCH	90-170	15	+ 1.7	-0.00**	+ 1.0**	+0.20**	+ 4.1	+0.34	0.46
16.04	*cis*-1,4-Di MCH	90-170	15	+ 2.1	-0.09**	+ 0.6**	+0.04**	+ 4.1	-0.04	0.40
16.05	*trans*-1,4-Di MCH	90-170	15	+ 1.6	-0.04**	+ 1.5**	+0.46	+ 4.7	+0.67	0.77
Cyclohexenes										
17.01	Cyclohexene	90-170	15	+ 4.4	-0.16**	+ 0.3**	+0.74	+ 7.1	+0.94	0.49
17.02	1,3-Cyclohexadiene	90-170	15	+ 6.5	-0.50*	+ 1.8**	+0.84*	+12.5	+0.62	0.62
17.03	1,4-Cyclohexadiene	90-170	15	+ 7.6	+0.26**	+ 0.3**	-0.12**	+11.9	+0.32	0.53

No.	Thermodynamic data : C78 / PSH								
	PSH - C78			Mixture		id([SH] =1) - C78			σ
	ΔH	ΔS	ΔC_P	h	s	$\acute{\Delta}H$	$\acute{\Delta}S$	$\acute{\Delta}C_P$	
	(cal mol^{-1})	(cal $mol^{-1}K^{-1}$)		(cal mol^{-1})	(cal mol^{-1} K^{-1})	(cal l mol^{-2})	(cal l $mol^{-2}K^{-1}$)		(cal mol^{-1})
1-Alkynes									
12.05	+ 20*	-0.068^{s}	-2.9	-159	-0.476	- 234	-0.864	-4.6	1.4
12.06	+ 14**	-0.097	-0.5**	-139	-0.472	- 223	-0.921	-1.2	1.3
12.07	+ 41	-0.044**	-1.6**	- 2**	-0.159**	+ 2	-0.420	-2.5	1.7
12.08	+ 66	-0.003**	-0.3**	- 23**	-0.264^{s}	- 4	-0.541	-0.7	1.6
12.09	+103	+0.071*	-0.2**	+ 87**	-0.042**	+ 193	-0.149	-0.3	2.0
12.10	+103	+0.057	-1.6	+195	+0.211	+ 340	+0.175	-2.1	1.6
Alkynes									
13.01	+ 31*	-0.084^{s}	+0.3**	+ 56**	-0.009**	+ 70	-0.265	+0.3	1.9
13.02	- 3**	-0.163	-2.1	+110	+0.128*	+ 98	-0.183	-3.1	0.9
13.03	+ 44	-0.088	-2.2^{s}	+165	+0.179*	+ 221	-0.059	-3.1	1.4
Monocyclic hydrocarbons									
14.05	+ 2**	-0.182	-2.2**	- 42**	-0.256*	- 117	-0.772	-3.5	2.2
14.06	+ 50	-0.089	-0.5**	+141	+0.167^{s}	+ 202	-0.060	-0.7	0.9
14.07	+112	+0.058**	-0.4**	+176	+0.183**	+ 326	+0.138	-0.5	1.9
14.08	+197	+0.258	-1.5**	+266	+0.360*	+ 562	+0.642	-2.4	2.9
14.10	+224^{s}	+0.292**	-1.4**	+141**	-0.017**	+ 408	+0.117	-1.9	3.0
Bicyclic hydrocarbons									
15.01	+103**	+0.007**	+1.5**	+167*	+0.086**	+ 284	-0.114	+2.1	2.7
15.02	+198^{s}	+0.216**	+0.8**	+260	+0.291**	+ 542	+0.451	+1.4	2.7
15.03	+236*	+0.319**	-0.6**	+226*	+0.193**	+ 545	+0.453	-0.6	3.9
15.04	+176*	+0.162**	-0.4**	+253^{s}	+0.238^{s}	+ 493	+0.282	-0.4	3.5
Methylcyclohexanes (MCH)									
16.01	+ 66	-0.077*	-0.3**	+172^{s}	+0.212**	+ 259	-0.005	-0.4	2.4
16.02	+ 68	-0.076^{s}	+2.3*	+173	+0.182**	+ 258	-0.057	+3.3	1.7
16.03	+ 88	-0.034**	+1.1**	+133^{s}	+0.099**	+ 231	-0.114	+1.5	2.0
16.04	+ 76	-0.061*	+2.1*	+ 94*	+0.001**	+ 159	-0.289	+2.8	1.7
16.05	+ 84	-0.044**	+2.8**	+173*	+0.213**	+ 285	+0.043	+4.0	3.3
Cyclohexenes									
17.01	+ 30**	-0.119*	-0.0**	+209^{s}	+0.327*	+ 272	+0.129	+0.1	2.9
17.02	- 26*	-0.239	+2.1*	+145	+0.196**	+ 114	-0.198	+2.9	1.8
17.03	+ 48*	-0.043**	+2.0**	+127**	+0.118**	+ 187	-0.045	+2.8	2.9

(Continued on pages 426 and 427)

Table 10 (*continued*)

No.	*Compound*	*Temp. range* (°C)	*n*	*Retention index : C78 / PSH*						
				PSH- C78		*Mixture*		*id([SH] =1) - C78*		σ
				ΔI_{130}	$10 \times \Delta A_T$ (K^{-1})	A_L	$10 \times A_{LT}$ (K^{-1})	$\Delta I'_{130}$ ($l\ mol^{-1}$)	$10 \times \Delta A'_T$ ($K^{-1} l\ mol^{-1}$)	
Alkylbenzenes										
18.00	Benzene	90-170	15	+ 9.7	+0.76	+ 0.1**	-0.30**	+14.8	+0.83	0.34
18.01	Toluene	90-170	15	+ 9.7	+0.85	+ 0.9**	-0.22**	+16.0	+1.09	0.38
18.02	Ethylbenzene	90-170	15	+ 9.9	+0.82	- 0.2**	+0.78s	+14.8	+2.54	0.43
Miscellaneous										
19.01	Adamantane	130-210	15	+ 5.8	+1.18	+ 2.5**	-0.07**	+12.6	+1.78	1.23
19.02	Naphthalene	130-210	15	+18.6	+0.70	+ 8.4s	-1.09**	+40.5	-0.22	1.12
19.03	Azulene	130-210	15	+21.4	+1.36	+ 5.8	+0.14	+41.1	+2.63	1.91
ALKANE DERIVATIVES										
1-Fluoroalkanes										
20.05	1-Fluoropentane	90-170	15	+ 6.0	-0.91	+ 0.2**	-0.56**	+ 9.2	-2.13	0.46
20.06	1-Fluorohexane	90-170	15	+ 6.9	-0.27s	+ 1.6	-0.36*	+12.7	-0.83	0.28
20.07	1-Fluoroheptane	90-170	15	+ 6.9	-0.13	+ 1.9	-0.10**	+13.2	-0.23	0.11
20.08	1-Fluorooctane	90-170	15	+ 7.1	-0.19**	+ 2.9	+0.42*	+15.1	+0.48	0.31
1,1,1-Trifluoroalkanes										
21.08	1,1,1-Trifluorooctane	90-170	15	+ 2.9	-0.18**	+ 3.6	+0.66**	+ 9.8	+0.81	0.56
21.10	1,1,1-Trifluorodecane	90-170	15	+ 2.9	-0.53s	+ 2.7	+0.70*	+ 8.4	+0.33	0.53
1-Chloroalkanes										
22.04	1-Chlorobutane	90-170	15	+ 8.8	-0.14**	+ 0.2**	-0.40*	+13.5	-0.69	0.31
22.05	1-Chloropentane	90-170	15	+ 8.9	+0.66	+ 0.4**	-0.22**	+14.0	+0.79	0.39
22.06	1-Chlorohexane	90-170	15	+ 9.0	+0.50	+ 1.4**	+0.16**	+15.7	+1.13	0.49
1-Bromoalkanes										
23.03	1-Bromopropane	90-170	15	+11.2	+0.40**	+ 1.5**	-0.92**	+19.0	-0.61	1.15
23.04	1-Bromobutane	90-170	15	+10.8	+0.41**	+ 2.5*	-0.12**	+20.0	+0.62	0.79
23.05	1-Bromopentane	90-170	15	+10.8	+0.32**	+ 2.7**	+0.14**	+20.3	+0.88	0.97
1-Cyanoalkanes										
24.02	Cyanoethane	90-170	15	+28.0	+0.07**	+15.6	-0.90**	+60.5	-0.52	0.85
24.03	1-Cyanopropane	90-170	15	+23.9	+0.77	+13.3	-0.94s	+55.9	+0.25	0.49
24.04	1-Cyanobutane	90-170	15	+24.2	+1.08	+10.9	-0.80**	+52.8	+0.89	0.65
24.05	1-Cyanopentane	90-170	15	+24.6	+1.13	+10.6	-0.72*	+52.9	+1.09	0.45

No.	Thermodynamic data : C78 / PSH								
	PSH - C78			Mixture		id([SH] =1) - C78			σ
	ΔH (cal mol^{-1})	ΔS (cal mol^{-1}K^{-1})	ΔCp (cal mol^{-1}K^{-1})	h (cal mol^{-1})	s (cal mol^{-1} K^{-1})	Δ'H (cal l mol^{-2})	Δ'S (cal l mol^{-2}K^{-1})	Δ'Cp (cal l mol^{-2}K^{-1})	(cal mol^{-1})
Alkylbenzenes									
18.00	+ 73	+0.059*	+0.4**	+179	+0.261^{s}	+ 305	+0.324	+0.8	1.8
18.01	+ 87	+0.083	-3.1	+225	+0.346	+ 381	+0.455	-4.1	1.1
18.02	+ 91	+0.078*	-2.6*	+445	+0.841	+ 688	+1.124	-3.0	1.9
Miscellaneous									
19.01	+109	+0.039	+2.5	+ 81**	-0.118**	+ 176	-0.345	+3.4	4.4
19.02	- 52**	-0.218**	+1.5**	-121**	-0.579*	- 309	-1.288	+1.4	4.7
19.03	-122**	-0.363**	+5.2**	+116**	-0.063**	- 76	-0.773	+6.9	8.6
ALKANE DERIVATIVES									
1-Fluoroalkanes									
20.05	- 79	-0.334	-1.3**	-245	-0.741	- 508	-1.646	-2.7	1.9
20.06	- 1**	-0.160	+1.6*	- 54**	-0.286	- 131	-0.764	+1.9	1.2
20.07	+ 22	-0.113	-0.4**	+ 46	-0.072*	+ 35	-0.416	-0.8	0.6
20.08	+ 23*	-0.124	-1.6**	+147	+0.151**	+ 172	-0.134	-2.3	1.5
1,1,1-Trifluroalkanes									
21.08	+ 60	-0.068**	+1.3**	+178	+0.287*	+ 274	+0.154	+1.9	2.4
21.10	+ 43*	-0.136^{s}	-1.0**	+154*	+0.143**	+ 195	-0.199	-1.5	2.9
1-Chloroalkanes									
22.04	- 16**	-0.162	-1.3**	- 30**	-0.239^{s}	- 116	-0.696	-2.2	1.4
22.05	+ 77	+0.055*	-2.6	+191	+0.269	+ 320	+0.309	-3.5	1.4
22.06	+ 66	+0.015**	-3.7	+237	+0.359	+ 362	+0.362	-5.0	1.4
1-Bromoalkanes									
23.03	+ 9**	-0.054**	-6.9^{s}	- 45**	-0.256**	- 94	-0.548	-9.1	4.2
23.04	+ 27*	-0.038**	-4.8	+135^{s}	+0.162	+ 178	+0.048	-6.8	1.9
23.05	+ 24**	-0.059	-6.4	+179^{s}	+0.238**	+ 227	+0.103	-8.9	2.6
1-Cyanoalkanes									
24.02	-197	-0.309	-4.2*	-254	-0.477	- 576	-0.928	-6.7	3.3
24.03	- 86	-0.132	+2.9	-108^{s}	-0.228^{s}	- 252	-0.454	+3.8	1.5
24.04	- 36^{s}	-0.038**	+3.2	+ 27**	+0.019**	- 10	-0.019	+4.5	1.7
24.05	- 29^{s}	-0.031**	+1.7*	+ 79*	+0.103**	+ 63	+0.083	+2.5	1.4

(*Continued on pages 428 and 429*)

Table 10 (*continued*)

No.	Compound	Temp. range	n	Retention index : C78 / PSH						
				PSH- C78		Mixture		id([SH] =1) - C78		σ
		(°C)		ΔI_{130}	10 × ΔA_T (K^{-1})	A_L	10 × A_{LT} (K^{-1})	ΔI_{130} ($l\ mol^{-1}$)	10 × ΔA_T ($K^{-1} l\ mol^{-1}$)	
1-Nitroalkanes										
25.02	Nitroethane	90-170	15	+25.0	+0.33	+ 8.1	-1.50	+49.6	-1.31	0.30
25.03	1-Nitropropane	90-170	15	+23.2	+0.37[s]	+ 8.1	-1.10	+46.9	-0.67	0.38
25.04	1-Nitrobutane	90-170	15	+23.0	+0.48	+ 7.0	-0.70*	+45.1	+0.08	0.44
25.05	1-Nitropentane	90-170	15	+22.8	+0.88	+ 7.6	-1.00*	+45.7	+0.23	0.79
1-Acetoxyalkanes										
26.03	1-Acetoxypropane	90-170	15	+11.7	-0.37	+ 4.2	-0.04**	+23.9	-0.40	0.28
26.04	1-Acetoxybutane	90-170	15	+11.5	-0.18	+ 3.0	+0.10**	+21.8	+0.08	0.17
26.05	1-Acetoxypentane	90-170	15	+11.2	-0.15*	+ 3.2	+0.00**	+21.6	-0.03	0.22
1-Alkanols										
27.04	1-Butanol	90-170	15	+19.0	-0.66	+29.0	-1.72	+71.9	-2.93	0.25
27.05	1-Pentanol	90-170	15	+18.3	-0.05**	+23.9	-1.48	+63.3	-1.73	0.37
27.06	1-Hexanol	90-170	15	+18.3	-0.12**	+21.5	-1.90	+59.6	-2.49	0.41
27.07	1-Heptanol	90-170	15	+18.4	+0.39*	+22.2	-2.54	+60.8	-2.68	0.58
2-Alkanols										
28.04	2-Butanol	90-170	15	+15.5	-0.14**	+17.9	-1.16*	+50.1	-1.50	0.77
28.05	2-Pentanol	90-170	15	+15.3	+0.46**	+16.9	-0.72**	+48.4	+0.05	0.87
28.06	2-Hexanol	90-170	15	+15.5	+0.24**	+15.0	-0.40**	+45.8	+0.17	0.76
28.07	2-Heptanol	90-170	15	+15.7	+0.20**	+12.9	+0.04**	+43.0	+0.75	0.51
2-Methyl-2-alkanols										
29.04	2-Methyl-2-propanol	90-170	15	+12.0	-1.33	+14.3	+0.34**	+39.4	-1.13	1.07
29.05	2-Methyl-2-butanol	90-170	15	+12.7	-0.67	+ 9.7	-0.52**	+33.5	-1.49	0.56
29.06	2-Methyl-2-pentanol	90-170	15	+13.1	-0.45**	+ 9.2	-0.46**	+33.4	-1.07	0.77
29.07	2-Methyl-2-hexanol	90-170	15	+12.7	-0.42	+ 8.4	-0.36**	+31.6	-0.89	0.36
1-Alkanethiols										
30.04	1-Butanethiol	90-170	15	+10.4	-1.47	- 0.3**	-0.66**	+14.9	-3.07	1.11
30.05	1-Pentanethiol	90-170	15	+11.4	-1.12	+ 1.2*	-0.28**	+18.8	-1.94	0.36
30.06	1-Hexanethiol	90-170	15	+11.7	-0.42**	+ 1.2**	-1.04*	+19.2	-2.02	0.77
2-Alkanones										
31.04	2-Butanone	90-170	15	+17.6	-1.61	+ 8.2	-1.42	+38.5	-4.21	0.63
31.05	2-Pentanone	90-170	15	+16.6	-0.95	+ 6.0	-0.78[s]	+33.8	-2.29	0.46

No.	Thermodynamic data : C78 / PSH								
	PSH - C78			Mixture		id([SH] =1) - C78			σ
	ΔH (cal mol^{-1})	ΔS (cal $mol^{-1}K^{-1}$)	ΔC_p (cal $mol^{-1}K^{-1}$)	h (cal mol^{-1})	s (cal mol^{-1} K^{-1})	$\Delta H'$ (cal l mol^{-2})	$\Delta S'$ (cal l $mol^{-2}K^{-1}$)	$\Delta C_p'$ (cal l $mol^{-2}K^{-1}$)	(cal mol^{-1})
1-Nitroalkanes									
25.02	-129	-0.202	-0.3**	-269	-0.697	- 550	-1.239	-1.1	1.9
25.03	-105	-0.200	-1.0**	-152*	-0.448	- 368	-0.927	-1.9	2.2
25.04	- 81	-0.159	-2.9	- 15**	-0.161	- 153	-0.495	-4.4	1.6
25.05	- 34**	-0.062**	-4.4*	+ 17**	-0.116**	- 51	-0.319	-6.4	3.4
1-Acetoxyalkanes									
26.03	- 61	-0.242	+1.4**	- 28**	-0.182*	- 161	-0.688	+1.6	1.5
26.04	- 28	-0.179	+0.7**	+ 67	-0.001**	+ 8	-0.374	+0.8	0.8
26.05	- 15*	-0.163	-1.5*	+ 64*	-0.044**	+ 11	-0.438	-2.4	1.0
1-Alkanols									
27.04	-181	-0.436	+2.1*	-731	-1.576	-1 250	-2.747	+1.4	1.2
27.05	- 92	-0.245	+0.8**	-463	-1.032	- 771	-1.770	+0.1	2.1
27.06	- 91	-0.259	+0.2**	-520	-1.245	- 866	-2.132	-0.9	2.4
27.07	- 31**	-0.120*	-3.4*	-539	-1.320	- 817	-2.063	-5.9	3.0
2-Alkanols									
28.04	- 88*	-0.226*	-0.7**	-398	-0.873*	- 672	-1.517	-1.8	4.9
28.05	- 11**	-0.074**	+1.4**	-147**	-0.315**	- 223	-0.549	+1.7	4.2
28.06	- 26**	-0.126*	+0.8**	- 87**	-0.232**	- 174	-0.541	+0.8	3.7
28.07	- 27**	-0.138*	-1.0**	+ 31**	-0.006**	- 22	-0.273	-1.6	2.7
2-Methyl-2-alkanols									
29.04	-193	-0.524	+0.0**	-294*	-0.638**	- 684	-1.631	-0.9	6.5
29.05	-121	-0.370	+1.5**	-294	-0.750	- 604	-1.628	+1.2	3.1
29.06	- 81	-0.289	+4.2*	-193*	-0.544	- 413	-1.242	+5.3	2.7
29.07	- 64	-0.259	-0.1**	-137*	-0.455	- 323	-1.107	-0.7	2.0
1-Alkanethiols									
30.04	-163	-0.519	-0.7**	-341*	-1.041*	- 771	-2.351	-2.3	5.5
30.05	-126	-0.437	+0.9**	-190	-0.689	- 508	-1.746	+0.3	1.8
30.06	- 49*	-0.253	-2.5	-191*	-0.726	- 410	-1.561	-4.4	3.7
2-Alkanones									
31.04	-272	-0.657	+1.5**	-686	-1.715	-1 359	-3.366	+0.2	3.9
31.05	-176	-0.461	+1.4	-338	-0.921	- 748	-2.001	+0.9	2.6

(Continued on pages 430 and 431)

Table 10 (*continued*)

No.	Compound	Temp. range (°C)	n	Retention index : C78 / PSH						
				PSH- C78		Mixture		id([SH] = 1) - C78		σ
				ΔI_{130}	10 × ΔA_T (K^{-1})	A_L	10 × A_{LT} (K^{-1})	ΔI_{130} (l mol^{-1})	10 × ΔA_T (K^{-1}l mol^{-1})	
31.06	2-Hexanone	90-170	15	+16.9	-0.71	+ 5.8	-0.62*	+33.9	-1.69	0.49
31.07	2-Heptanone	90-170	15	+17.1	-0.62	+ 5.8	-0.44**	+34.3	-1.28	0.47
Aldehydes										
32.05	Pentanal	90-170	15	+15.7	+0.07**	+ 7.0	-1.28	+33.9	-1.51	0.43
32.06	Hexanal	90-170	15	+16.2	+0.34s	+ 6.0	-0.76s	+33.3	-0.33	0.37
32.07	Heptanal	90-170	15	+16.5	+0.41	+ 6.1	-0.79	+33.8	-0.32	0.31
Ethers										
33.06	Dipropylether	90-170	15	+ 4.1	-0.45*	+ 1.1**	-0.82*	+ 7.7	-1.84	0.59
33.08	Dibutylether	90-170	15	+ 4.0	-0.22s	+ 1.2	-0.94	+ 7.7	-1.68	0.24
Halomethanes										
37.01	Dichloromethane	90-170	15	+13.1	+0.78s	+ 6.8	+0.76**	+30.1	+2.59	0.78
37.02	Trichloromethane	90-170	15	+12.3	+0.56	+ 4.2	-0.16**	+24.8	+0.83	0.53
37.03	Tetrachloromethane	90-170	15	+ 5.7	+0.03**	+ 0.1**	-0.24**	+ 8.7	-0.24	0.40
37.04	CF_2Br_2	90-170	15	+ 4.3	-0.10**	+ 5.6	+1.38	+15.0	+2.06	0.32
HALOBENZENES										
38.01	Fluorobenzene	90-170	15	+ 9.9	+0.29*	+ 1.5*	+0.08**	+17.2	+0.71	0.44
38.02	Hexafluorobenzene	90-170	15	+ 2.1	-0.72	+ 6.3	+2.40	+12.8	+2.64	0.52
38.03	Trifluoromethylbenzene	90-170	15	+ 7.4	+0.10**	+ 2.6*	+1.74	+15.2	+2.90	0.81
38.04	Chlorobenzene	90-170	15	+12.3	+0.72	+ 1.5**	+0.38**	+20.9	+1.84	0.53
38.05	Bromobenzene	90-170	15	+14.7	+0.98	+ 2.6*	-0.12**	+26.1	+1.53	0.72
38.06	Iodobenzene	130-210	15	+16.8	+1.19	+ 3.4*	+0.85s	+30.6	+3.34	0.49
ALKYLPYRIDINES										
39.01	Pyridine	90-170	15	+19.1	+0.59	+ 7.2	-1.20	+39.5	-0.56	0.48
39.02	2-Picoline	90-170	15	+16.5	+0.79	+ 4.0	-0.84	+30.8	+0.20	0.34
39.03	3-Picoline	90-170	15	+20.1	+0.91	+ 8.8	-0.88	+43.5	+0.44	0.34
39.04	4-Picoline	90-170	15	+20.0	+0.49	+ 7.5	-0.94	+41.3	-0.30	0.28
39.05	2,3-Lutidine	130-210	15	+18.2	+0.59	+ 2.9s	+1.06	+31.9	+2.77	0.34
39.06	2,4-Lutidine	130-210	15	+17.2	+0.52	+ 4.5	+0.40s	+32.7	+1.68	0.24
39.07	2,5-Lutidine	130-210	15	+15.8	+0.98	+ 2.9*	+1.51	+28.4	+4.00	0.75
39.08	2,6-Lutidine	130-210	15	+16.3	-0.25	+ 5.0	-0.14**	+31.9	-0.29	0.24

No.	Thermodynamic data : C78 / PSH								
	PSH - C78			Mixture		id([SH] =1) - C78			σ
	ΔH (cal mol-1)	ΔS (cal mol-1K-1)	ΔCp (cal mol-1K-1)	h (cal mol-1)	s (cal mol-1 K-1)	Δ'H (cal l mol-2)	Δ'S (cal l mol-2K-1)	Δ'Cp (cal l mol-2K-1)	(cal mol-1)
31.06	-141	-0.338	+0.6**	-233	-0.704	- 559	-1.621	-0.0	2.8
31.07	-126	-0.365	-0.2**	-161s	-0.562	- 445	-1.410	-1.1	2.7
Aldehydes									
32.05	- 62	-0.186	-1.7**	-244	-0.683	- 455	-1.285	-3.1	2.4
32.06	- 27*	-0.112	-2.3*	- 46**	-0.247s	- 136	-0.591	-3.6	1.7
32.07	- 28*	-0.108	-1.9*	- 45**	-0.204s	- 109	-0.430	-2.7	2.1
Ethers									
33.06	+ 5**	-0.173	-1.4**	-183*	-0.612	- 314	-1.266	-2.7	3.2
33.08	+ 50	-0.094	-1.4s	-122	-0.531	- 181	-1.083	-2.6	0.9
Halomethanes									
37.01	+ 33**	+0.044**	+0.1**	+340s	+0.812s	+ 518	+1.187	+0.8	4.7
37.02	+ 19**	-0.031**	+0.7**	+116**	+0.183**	+ 160	+0.138	+1.1	3.2
37.03	+ 35*	-0.087*	+1.0**	+ 38**	-0.089**	+ 42	-0.402	+1.2	2.3
37.04	+ 21**	-0.104	+0.8**	+295	+0.695	+ 416	+0.758	+1.6	1.7
HALOBENZENES									
38.01	+ 22**	-0.064**	+1.4**	+151s	+0.215**	+ 198	+0.097	+2.1	2.5
38.02	- 11**	-0.225	+1.5**	+407	+0.958	+ 520	+0.937	+2.7	2.8
38.03	+ 31**	-0.072**	+1.0**	+470	+1.019	+ 661	+1.219	+2.1	4.8
38.04	+ 53*	+0.014**	-0.7**	+320	+0.557s	+ 468	+0.657	-0.6	3.1
38.05	+ 62*	+0.050**	-1.7**	+265s	+0.401**	+ 401	+0.483	-2.1	4.0
38.06	+135*	+0.238**	-0.7**	+231	+0.285*	+ 452	+0.576	-0.7	2.4
ALKYLPYRIDINES									
39.01	- 36*	-0.099*	-0.4**	-115**	-0.393*	- 235	-0.750	-1.0	2.8
39.02	+ 14**	-0.023**	+0.1**	+ 44**	-0.068**	+ 42	-0.230	+0.0	1.8
39.03	- 5**	-0.032**	-0.5**	+ 18**	-0.087**	- 8	-0.235	-0.8	1.9
39.04	- 48	-0.138	-0.4**	- 68**	-0.317	- 194	-0.719	-1.0	1.6
39.05	+ 27**	+0.010**	-0.3**	+275	+0.443	+ 377	+0.516	-0.1	1.8
39.06	- 21**	-0.115s	+0.9*	+148	+0.152	+ 133	-0.066	+1.3	0.7
39.07	- 29**	-0.146**	+3.3*	+348	+0.629	+ 402	+0.559	+5.0	2.4
39.08	-149	-0.436	+1.2**	+ 52**	-0.063**	- 182	-0.818	+1.3	1.1

(Continued on pages 432 and 433)

Table 10 (*continued*)

No.	Compound	Temp. range (°C)	n	Retention index : C78 / PSH — PSH- C78 ΔI_{130}	PSH- C78 $10 \times \Delta A_T$ (K^{-1})	Mixture A_L	Mixture $10 \times A_{LT}$ (K^{-1})	id([SH] =1) - C78 ΔI_{130} $(l\ mol^{-1})$	id([SH] =1) - C78 $10 \times \Delta A_T$ $(K^{-1} l\ mol^{-1})$	σ
39.09	3,4-Lutidine	130-210	15	+23.8	-0.04**	+10.0	-0.48**	+50.8	-0.32	0.49
39.10	3,5-Lutidine	130-210	15	+22.4	-0.09**	+ 9.5	-0.66	+47.9	-0.69	0.32
39.11	2-Ethylpyridine	130-210	15	+15.2	+0.17**	+ 2.3**	+0.52**	+26.4	+1.28	0.65
39.12	3-Ethylpyridine	130-210	15	+17.2	-0.09**	+ 2.3**	-1.22	+29.2	-1.71	0.45
39.13	4-Ethylpyridine	130-210	15	+18.9	+0.28**	+ 1.5**	+1.33*	+30.8	+2.69	1.07
39.14	2-Propylpyridine	130-210	15	+14.4	-0.05**	+ 3.5**	-0.62**	+26.8	-0.77	0.80
39.15	4-Propylpyridine	130-210	15	+18.2	+0.92	+ 5.2	+1.06	+35.4	+3.29	0.45
39.16	2,3,6-Collidine	130-210	15	+15.0	+0.25	+ 3.4^{s}	+0.17**	+27.7	+0.88	0.41
39.17	2,4,6-Collidine	130-210	15	+14.1	+0.20*	+ 8.3	-1.25	+33.6	-1.28	0.61
39.18	4-*tert*-Butylpyridine	130-210	15	+19.1	-0.16**	+ 4.6^{s}	-0.35**	+35.6	-0.45	0.62
39.19	3-Chloropyridine	90-170	15	+17.1	+0.49	+ 5.4	+0.04**	+33.9	+1.10	0.54
	ORGANOSILICON COMPOUNDS									
40.01	Tetramethylsilane	90-170	15	+ 0.3*	+0.14	+ 2.9	+0.26**	+ 4.3	+1.00	0.28
40.02	Hexamethyldisilane	90-170	15	- 1.8	-0.09**	- 0.6**	+0.28**	- 3.6	+0.25	0.31
40.03	Hexamethyldisiloxane	90-170	15	- 4.6	-0.89	- 0.8**	+1.58^{s}	- 8.0	+0.97	0.87
	MISCELLANEOUS									
41.01	Carbon disulphide	90-170	15	+ 8.1	+0.59	+ 1.3^{s}	-1.56	+14.0	-1.33	0.30
41.02	Tetramethyltin	90-170	15	+ 0.8	+0.73	- 1.5	+0.38*	- 0.9	+1.67	0.26
41.03	Tetrahydrofuran	90-170	15	+12.4	-0.55^{s}	+ 7.3	+0.30**	+29.6	-0.11	0.66
41.04	1,4-Dioxane	90-170	15	+14.2	-0.16**	+ 5.3	+0.24**	+29.3	+0.39	0.83
41.05	Thiophene	90-170	15	+11.1	+1.31	+ 1.9**	+0.66**	+19.8	+3.14	0.90
41.06	Cyclopentanone	90-170	15	+20.6	-0.26**	+ 7.5	-0.02**	+42.2	-0.04	0.74
41.07	Cyclohexanone	90-170	15	+21.7	+0.99	+ 7.2	-0.40**	+43.5	+1.28	0.73
41.08	Cyclohexanol	90-170	15	+19.0	-0.18**	+14.2	-0.18**	+49.9	-0.09	1.10
41.11	Nitrobenzene	130-210	15	+24.8	+0.70	+16.0	-0.51**	+61.4	+0.84	0.74
41.12	Benzyl alcohol	130-210	15	+30.0	+0.40	+13.7	+2.24	+65.9	+4.56	0.54
41.13	2-Phenylethanol	130-210	15	+27.5	+0.36	+ 9.6	+2.14	+56.0	+4.26	0.54
41.14	Anisole	130-210	15	+27.9	+0.30	+20.6	+0.32	+68.4	+1.66	0.21
41.15	Phenetole	130-210	15	+23.0	+0.54	+19.8	+0.56	+64.5	+2.24	0.25
ERRORS:	*f (n-alkanes)*	*90-210*		*def.*						
	f (n-alkanes)	*150-210*		*def.*						
	f (solutes)	*90-170*		*0.63*	*0.22*	*2.19*	*0.77*	*3.21*	*1.13*	
	f (solutes)	*130-210*		*1.09*	*0.22*	*3.79*	*0.77*	*5.56*	*1.13*	
CONVERSION TO K_D:				*0*	*0*	*0*	*0*	*0*	*0*	

Table 10 (*continued*)

No.	*Thermodynamic data : C78 / PSH*								
	PSH - C78			*Mixture*		*id([SH] =1) - C78*			*σ*
	ΔH (cal mol^{-1})	*ΔS* (cal mol^{-1}K^{-1})	*ΔCp*	*h* (cal mol^{-1})	*s* (cal mol^{-1} K^{-1})	*ΔH'* (cal l mol^{-2})	*ΔS'* (cal l mol^{-2}K^{-1})	*ΔCp'*	(cal mol^{-1})
39.09	-202	-0.492	+1.6**	- 48**	-0.293*	- 383	-1.184	+1.6	2.4
39.10	-192	-0.481	+1.4*	- 80^{s}	-0.369	- 416	-1.281	+1.3	1.1
39.11	-157	-0.467	+3.3	+174	+0.202^{s}	- 27	-0.503	+4.4	1.4
39.12	- 75**	-0.256*	-0.4**	- 98*	-0.499	- 303	-1.214	-1.2	2.0
39.13	-188*	-0.506^{s}	+3.6**	+310	+0.514^{s}	+ 124	-0.109	+5.1	3.2
39.14	+ 33**	-0.034**	-2.1**	+ 1**	-0.249**	- 17	-0.564	-3.3	3.2
39.15	+ 47**	+0.046**	+0.8**	+264	+0.407	+ 387	+0.508	+1.4	1.7
39.16	- 36**	-0.194**	+0.9**	+137^{s}	+0.079**	+ 80	-0.319	+1.1	1.9
39.17	+ 41**	-0.017**	-1.1**	-144*	-0.556	- 202	-0.953	-2.1	2.9
39.18	-185^{s}	-0.523	+1.5**	+ 33**	-0.189**	- 273	-1.153	+1.5	2.7
39.19	- 90**	-0.279*	+2.4**	+ 67**	-0.027**	- 74	-0.538	+3.1	2.1
ORGANOSILICON COMPOUNDS									
40.01	+109	+0.066*	+0.7**	+137	+0.343	+ 315	+0.496	+1.3	1.7
40.02	+105	-0.007**	-1.5**	+148	+0.173*	+ 278	+0.034	-2.1	1.4
40.03	+ 33	-0.208	-2.1	+260	+0.479	+ 335	+0.185	-2.8	5.3
MISCELLANEOUS									
41.01	+ 52	-0.004**	+1.9**	-154	-0.519	- 191	-0.856	+2.2	1.9
41.02	+157	+0.169	-1.1	+340	+0.667	+ 636	+1.015	-1.0	1.3
41.03	- 97	-0.317	+1.1**	- 55**	-0.201**	- 240	-0.795	+1.1	3.6
41.04	- 69*	-0.234^{s}	+0.7**	+ 41**	-0.011**	- 70	-0.422	+0.8	4.6
41.05	+115	+0.172*	+2.7**	+482	+1.029	+ 801	+1.591	+4.7	4.3
41.06	-135	-0.330	+0.6**	- 52**	-0.240**	- 284	-0.855	+0.4	3.8
41.07	- 13**	-0.036**	+0.9**	+142**	+0.194**	+ 156	+0.156	+1.4	3.4
41.08	-104^{s}	-0.299	+3.1**	-125**	-0.378**	- 342	-1.003	+3.8	5.0
41.11	- 81**	-0.191**	+1.0**	- 88**	-0.346**	- 260	-0.812	+1.0	3.4
41.12	-245	-0.518	+3.2^{s}	+369	+0.798	+ 174	+0.392	+4.8	2.0
41.13	- 50**	-0.088**	-1.8**	+395	+0.780	+ 460	+0.909	-2.0	2.7
41.14	-101	-0.182^{s}	-0.7**	- 73^{s}	-0.123*	- 226	-0.380	-1.2	1.1
41.15	- 65*	-0.161*	+0.8**	+ 41**	+0.056**	- 41	-0.167	+1.0	1.2
E(contd)	*5.2*	*0.0128*	*0.17*	*4.3*	*0.0102*	*9.5*	*0.0231*	*0.24*	
	5.2	*0.0128*	*0.17*	*4.3*	*0.0102*	*9.5*	*0.0231*	*0.24*	
	9.1	*0.0224*	*0.76*	*31.3*	*0.0776*	*45.9*	*0.1139*	*1.07*	
	32.2	*0.0812*	*0.83*	*34.3*	*0.0775*	*66.3*	*0.1582*	*1.17*	
C(contd)	*- 3*	*-0.044*	*-0.1*	*- 1*	*-0.003*	*- 6*	*-0.066*	*-0.1*	

cal potential in the alkane C78, $\Delta\mu_j^{A}$, and the difference $\Delta'\mu_j^{P} = \Delta\mu_j^{P} - \Delta\mu_j^{A}$ at a given composition by Eq. (9)

$$m_j^{A/P} = a + b\,\Delta\mu_j^{A} + c\,\Delta'\mu_j^{P} \tag{9}$$

where the experimental value of the constant was calculated with data h_j and s_j listed in Tables 8–10, with Eq. (10)

$$m_j^{A/P} = h_j - Ts_j \tag{10}$$

The numerical values of the coefficients in Eq. (9) are as follows

	a	b	c	corr. coeff.: r
TMO	23.8	−0.0055	0.509	0.972
PCN	27.2	−0.0039	0.378	0.962
PSH	22.4	−0.0292	0.521	0.872

Calculated values of the constant, $m_j^{A/P}$, as a function of those measured by experiment are plotted in Figs. 3, 4 and 5. Assuming that for a given A/P-mixture the values of the coefficients are independent of the solute, j, the $\Delta'\mu$-value of an unknown solute can be estimated as described in Ref. [4].

The aim of the project stated in part I is the selection of a series of solvents where each solvent provides new information about interaction forces between the solute, j, and an interacting group, X. Let us characterize the additional interaction between j and X by its $\Delta'I$-value (analogous to the $\Delta'\mu$-value), i.e. the retention index difference between the index measured in a one molar ideal solution of X in C78 and the index in pure C78. Obviously, if

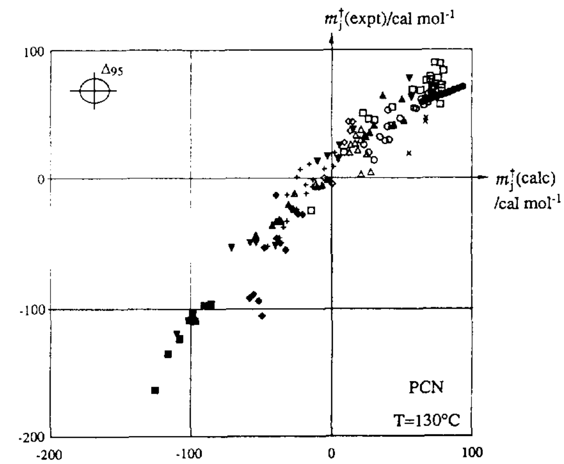

Fig. 4. Plot of the experimental constant, $m_j^{A/P}$ in Eq. (10), characterising the non-ideality of C78/PCN mixtures as a function of those calculated with Eq. (9) at 130°C.

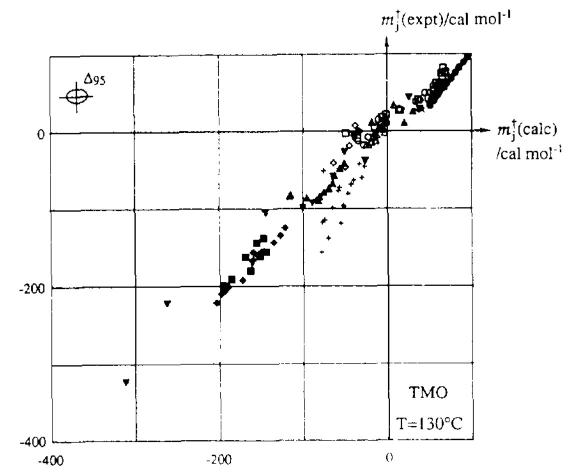

Fig. 3. Plot of the experimental constant, $m_j^{A/P}$ in Eq. (10), characterising the non-ideality of C78/TMO mixtures as a function of those calculated with Eq. (9) at 130°C.

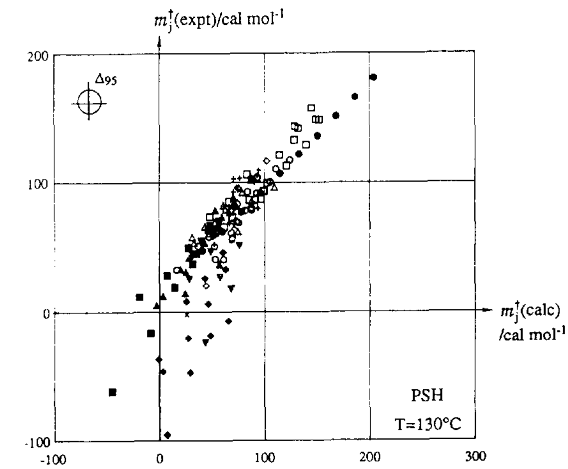

Fig. 5. Plot of the experimental constant, $m_j^{A/P}$ in Eq. (10), characterising the non-ideality of C78/PSH mixtures as a function of those calculated with Eq. (9) at 130°C.

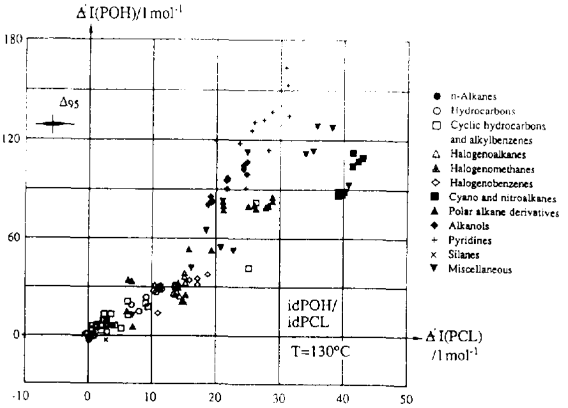

Fig. 6. Retention index difference of solutes in a hypothetical ideal one molar solution of the interacting groups POH in C78 as a function of the same difference in PCL and C78 ($\Delta' I$-values).

$\Delta' I$-values on two ideal solvents correlate, one of the solvents can be excluded from the family. In the last five figures $\Delta' I$-values on primary hydroxyl (POH), trifluoromethylalkane (CF_3) from Refs. [1] and [4] as well as methoxyalkane (MeO), primary cyano (PCN) and primary thiol (PSH) data are plotted as a function of $\Delta' I$-values on a one molar ideal solution of primary

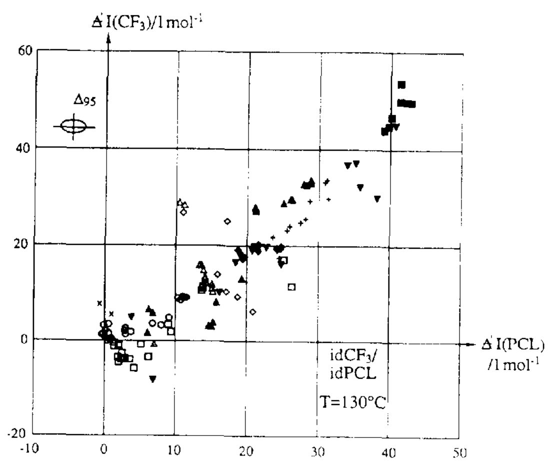

Fig. 7. Retention index difference of solutes in a hypothetical ideal one molar solution of the interacting groups CF_3 in C78 as a function of the same difference in PCL and C78 ($\Delta' I$-values).

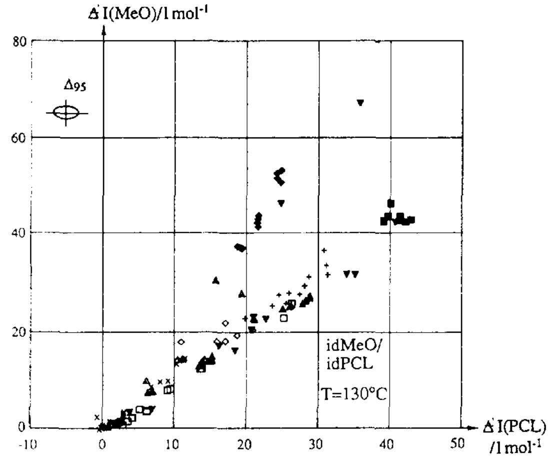

Fig. 8. Retention index difference of solutes in a hypothetical ideal one molar solution of the interacting groups MeO in C78 as a function of the same difference in PCL and C78 ($\Delta' I$-values).

chloroalkane (PCL) groups [5]. Latter was elected as standard as it approximates an ideal dipolar interacting group of average polarizability. In the following let us shortly comment on these figures:

– Primary hydroxyl can interact by its perma-

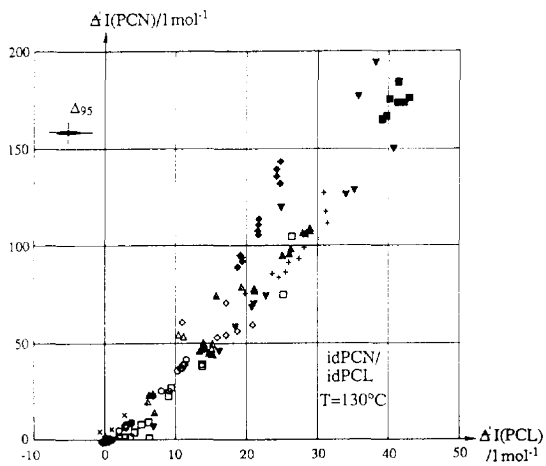

Fig. 9. Retention index difference of solutes in a hypothetical ideal one molar solution of the interacting groups PCN in C78 as a function of the same difference in PCL and C78 ($\Delta' I$-values).

nent polarity, and as a hydrogen bond donor and acceptor. Fig. 6 shows that alcohols, ethers, ketones etc. show a strong interaction.

– Trifluoromethylalkanes are similar to the primary chloroalkanes. Deviations in Fig. 7 were proposed to be due to the "hardness" of the trifluoromethyl group compared with the polariability of the chloro substituent [5].

– Methoxy groups can interact by permanent polarity and as hydrogen bond acceptors. Comparison of Fig. 8 with Fig. 6 shows that deviations are as awaited

– Cyano groups interact nearly exclusively by permanent polarity, they are weak hydrogen bond acceptors. In fact, in a "family of unlike solvents" this stationary phase might replace the PCL-solvent in which the chloro substituents are too reactive hence it cannot be used as stationary phase for certain solutes.

– The interaction forces of PSH groups are very interesting but for our purpose the behaviour of this phase is a deception. In fact, it was awaited that interaction forces between the slightly acidic thiol and basic compounds will be pronounced, i.e. that this phase measures the basicity of solutes. It is seen that pyridine derivatives are not retained more than other polar compounds. Interestingly this group is somewhat similar to the methoxy-alkane group. Fig. 10 shows that it seems to be a hydrogen bond acceptor and a very bad donor.

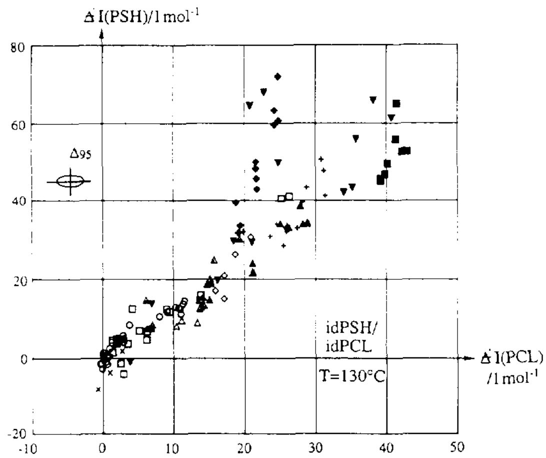

Fig. 10. Retention index difference of solutes in a hypothetical ideal one molar solution of the interacting groups PSH in C78 as a function of the same difference in PCL and C78 ($\dot{\Delta}'I$-values).

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References

[1] K.S. Reddy, J.-Cl. Dutoit and E. sz. Kováts, J. Chromatogr., 609 (1992) 229.

[2] K.S. Reddy and E. sz. Kováts, Chromatographia, 34 (1992) 249.

[3] R. Cloux, G. Défayes, K. Fóti, J.-Cl.Dutoit and E. sz. Kováts, Synthesis (1993) 909.

[4] K.S. Reddy, R. Cloux and E. sz. Kováts, J. Chromatogr. A, 673 (1994) 181.

[5] G. Défayes, K.S. Reddy, A. Dallos and E. sz. Kováts, J. Chromatogr. A, 699 (1995) 131.

[6] P. Zeltner, G.A. Huber, R. Peters, F. Tátrai, L. Boksányi and E. sz. Kováts, Helv. Chim. Acta, 62 (1979) 2495.

[7] M. Tamura and J.K. Kochi, Synthesis (1971) 303.

[8] G. Körösi and E. sz. Kováts, J. Chem. Eng. Data, 26 (1981) 323.

[9] R.A. Fisher and F. Yates, Statistical Tables, Oliver and Boyd, Edinburgh, 6th ed., 1963.