

Separation of an Industrial Mixture of Decalin or Naphthalene Fluorination Products: Cis-Perfluorodecalin, Trans-Perfluorodecalin and Perfluoro(butylcyclohexane): Physicochemical, Thermophysical, and Spectral Data

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Abstract: New physicochemical data for trans-perfluorodecalin (trans-PDF) and cis-perfluorodecalin (cis-PFD) are presented. Based on the differential scanning calorimetry, the temperature and heat of the solid–liquid phase transition are determined. The coefficients of Antoine’s equation are calculated based on the experimental temperature–pressure dependence data. This article also presents data on the rheological properties («zero» shear viscosity and apparent activation energy for the viscous flow) of the studied compounds. The dependencies of refractive index and excess volume (density) on temperature are studied. Gas chromatography–mass spectrometry data and FTIR, ¹³C NMR, and ¹⁹F NMR spectra are provided. The dependencies are given for the perfluoro(butylcyclohexane) (BCH)–trans-PFD, BCH–cis-PFD, and trans-PFD–cis-PFD binary systems and BCH–trans-PFD–cis-PFD ternary system: refractive index and density (liquid molar volume and excess molar volume) of composition and temperature. The dependences of the excess molar volume on the composition and temperature of the mixtures are correlated with Redlich-Kister and Kohler equations.

Keywords: trans-perfluorodecalin; cis-perfluorodecalin; perfluoro(butylcyclohexane); perfluorocycloalkanes; physicochemical data; saturated vapor pressure; density; refractive index; viscosity; excess molar volume

Citation: Lupachev, E.V.; Voshkin, A.A.; Kisel', A.V.; Kulov, N.N.; Zakhodyaeva, Y.A.; Polkovnichenko, A.V. Separation of an Industrial Mixture of Decalin or Naphthalene Fluorination Products: Cis-Perfluorodecalin, Trans-Perfluorodecalin and Perfluoro(butylcyclohexane): Physicochemical, Thermophysical, and Spectral Data. *Processes* **2023**, *11*, 3208. <https://doi.org/10.3390/pr11113208>

Academic Editor: Blaž Likozar

Received: 12 October 2023

Revised: 3 November 2023

Accepted: 8 November 2023

Published: 10 November 2023



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1. Introduction

According to macroeconomic projections in the Perfluorocarbons Market—Global Industry Analysis and Forecast (2023–2029) [1], the perfluorocarbons market is expected to grow at a compound annual growth rate of 4.2% during the forecast period, reaching US\$ 4.77 Bn by 2029. The report indicates that the perfluorocarbon (also called perfluoronaphthenes) application has facilitated the development of significantly more complex and faster processing semiconductors [1]. This will result in an increased demand for perfluorocarbons, considered major growth drivers for the market growth during the forecasted period. Meanwhile, application in the artificial photosynthesis process, which helps develop nanoemulsions for cancer detection, is attracting vendors. Perfluorocarbons are emerging in the healthcare sector and have been highly adopted in manufacturing as they help develop non-invasive imaging methodologies for assessing the potential efficacy of central nervous system transplantation of stem cells. Furthermore, development in the personal care and electronics sector is expected to serve as the primary growth factor for global perfluorocarbons in a calculated period. Semiconductor cleaning is a major

sector associated with its broad application and is, thus, broadly utilized to cover market value with significant growth.

The present research considers perfluorodecalin (PFD)–naphthalene, 1,1,2,2,3,3,4,4,4a,5,5,6,6,7,7,8,8,8a-octadecafluorodecahydro-. The history of PFD dates back to the 1940s. In the scientific literature, the over earlier mention of PFD application is associated with intravenous therapy [2]; until the 1990s, research on its use was mainly focused on blood substitution and oxygen carriers: oxygen-supply level after exchange blood-transfusion and liver function –mono-oxygenase system (cytochrome-P-450) microsomal cytochrome P-450-containing mono-oxygenase system [3–15]. PFD has also been considered as a matrix in spectroscopic studies [16], a chemical tracer to assess ocean models [17], and an aeration agent of the nutrient medium for tissue culture cell growth and mycobacteria culture [18,19].

An in-depth review of the scientific literature up to 2015 shown an active interest in PFD for myriad medical, biochemical, and chemical engineering side: blood substitute [20–24], liquid fluorocarbon lavage of airways [25–27], transplantology [28,29], extracorporeal life support [30], cryosurgery and tissue engineering [31–34], tattoos treatment [32,35–44], ophthalmology [45–55], drug production [56–60], headspace-gas chromatography-tandem [61] and electrospray ionization [62] mass spectrometry, magnetic resonance imaging oximetry [63], cell and microbial culturing [64–70], immersion medium [71–74], gas carrier and inert solvents [75–84], meso- and macro-mesoporous silica production [85], hydrogen production [86–88], and solar cell production [89].

Studies have also reported on various PFD properties: vapor pressure [90], phase data (LLE with hydrocarbon binary [91], ternary, etc. systems [92]); nucleation rate of gas hydrates [93,94], extraction [95], and gas solubility (liquid–gas partition-coefficients of halothane and isoflurane [96], N₂, N₂O, NH₃, O₂, and CO₂ [97–100]); density and viscosity [90,101–104]; surface properties (surface tension [104,105], interfacial tension against water [106], influence of pluronic F-68 dissolved in the aqueous phase [107], and wetting dynamics [108]); aqueous emulsions (preparation and physicochemical properties [109,110], effect of flocculation on particle enlargement [111]); adsorption properties [112] and aerodynamic diameter [113]; molecular structure and spectral properties (electron-diffraction of the gas phase structure [114], infrared spectra and radiative efficiency [115], NMR spectrum [63,116], conformation [117–120], and isomerization [121–124]); chemical and biological inertness of PFD [125–127]. Most data were obtained from a mixture of cis- and trans-PFD isomers (CAS No 306-94-5); many were not systematic and primarily related to PFD practical properties. Notably, the experimental data on the properties of PFD are especially relevant considering that the theoretical studies on the properties of fluorinated compounds are limited by the inability to apply the density functional theory (DFT) due to the relativistic effects and no overlap between the DFT exchange and exact exchange holes [128,129].

This article is a continuation of a series [130–134] on the separation and purification process of the constituents of the industrial system of close-boiling isomeric reaction products from the fluorination of decalin or naphthalene. The primary aim is to obtain physicochemical data on the properties of the cis- and trans-PFD isomers and their impurities: perfluoro(butylcyclohexane) (BCH). Note that physicochemical data on the pure substances and their mixtures are relatively absent from the literature. Such information is the foundation for developing separation/purification methods and is of significant scientific and industrial interest [130].

2. Materials and Methods

2.1. System and Its Component Data

The objects of this research are perfluoro-(butylcyclohexane), trans-perfluorodecalin, cis-perfluorodecalin (cis-PFD), and binary and ternary mixtures of these components. The considered components and their mixture are the constituents of an industrial system of

close-boiling geometric/configurational and structural/constitutional isomeric reaction products of the electrochemical fluorination of decalin or naphthalene [119,135,136]. Previously [130], we identified the main impurities of the reaction mixture (BCH and perfluoro(7-methylbicyclo[4.3.0]nonane) (MBCN)) and described the physicochemical properties of the BCH, MBCN and their binary mixture; the commercial value of BCH and MBCN was also discussed in previous works [130,131,133]. This study considers the BCH–trans-PFD–cis-PFD ternary constituent of the MBCN–BCH–trans-PFD–cis-PFD four-component industrial mixture.

The data on the compounds used are summarized in Table 1. BCH, cis- and trans-PFD were purified by distillation methods and crystallization. The purity of the reagents was confirmed by gas chromatography. The ¹H NMR additionally analyzed the samples to determine the partially fluorinated impurity content.

Table 1. Specifications of the compounds used.

| Chemical Name | CAS-No | Molar Mass M/g·mol ⁻¹ | Supplier | Initial Mass Fraction Purity | Purification Method | Mass Fraction after Purification (GC ^a) |
|-----------------------------|------------|-------------------------------------|------------|---------------------------------|---|---|
| Perfluoro(butylcyclohexane) | 374-60-7 | 500.07 | P&M Invest | 0.80–0.90 | Heteroazeotropic distillation and crystallization | ≥0.997 |
| Trans-perfluorodecalin | 60433-12-7 | 462.08 | P&M Invest | 0.80–0.90 | Heteroazeotropic distillation, crystallization | ≥0.998 |
| Cis-perfluorodecalin | 60433-11-6 | 462.08 | P&M Invest | 0.70–0.80 | Heteroazeotropic distillation, crystallization | ≥0.995 |

^a Gas chromatography–flame ionization detector (Agilent 6890N equipped with a Restek RTX-1701 RK12054 capillary column).

2.2. Equipment and Analytics

The molecular weights of cis-PFD and trans-PFD were determined by gas chromatograph Maestro- α MS (INTERLAB, Moscow, Russia) with a quadrupole mass spectrometer (capillary column SCI-5MS-025-025-30, UVISON, Sevenoaks, UK; vaporizer temperature (injection port temperature), 200 °C; column (oven) temperature, 40 °C (3 min); ionization energy, 70 eV; detector: scan mode, (m·z⁻¹ 50–550); interface temperature, 250 °C; ion source temperature, 230 °C; carrier gas–helium 1 mL·min⁻¹).

The Bruker AVANCE-300 radio spectrometer (Bruker, Billerica, MA, USA) and IRTracer-100 Spectrophotometer (Shimadzu, Kyoto, Japan) were used to obtain the nuclear magnetic resonance (NMR) and Fourier transform infrared (FTIR) spectra (Sigma-Aldrich St. Louis, MO, USA), respectively. Differential scanning calorimetry (DSC) was employed to determine the temperature and heat of the solid–liquid phase transition (METTLER TOLEDO DSC 3+, Mettler Toledo, Columbus, OH, USA). Rotational rheometry was used to study rheological properties (Anton Paar Physica MCR301 rheometer (Geminibv, Apeldoorn, Netherlands); stationary flow conditions). The Abbemat 3200 refractometer (Fisher Scientific, Hampton, NH, USA) and DMA 1001 densimeter (Anton Paar, Sumida City, Japan) were applied to measure refractive index, n_D , and density, ρ , respectively. A detailed description of the equipment and modes were described previously [130].

Mass Comparator MC-1000 (A&D Company, Limited Toshima City, Japan) was used to measure sample weight, m . Mercury “Mereno pri ponoru” thermometers and a vacuum meter VACUU VIE extended were also employed to measure temperature, T , and pressure, P , respectively.

2.3. Saturated Vapor Pressure Measurements

The saturated vapor pressure, P , was determined using the apparatus shown in Figure 1. The unit was hooded in a jacket to prevent partial condensation of vapors on the flask walls. After a constant pressure was set, the sample was brought to a boil with

continuous stirring (UT 4100S heating mantle (Trulia, San Francis, CA, USA) was used). The vapor phase produced in still 1 was condensed in the backflow condenser 2 and fed back to still 1. The vapor, T_D , and liquid, T_W , phase temperatures were measured using thermometers 3 and 4, respectively. The values were recorded once the parameters (T , P) were constant for 30 min. This was repeated three times for each experiment. The methodology was previously validated with distilled water [130] and is similar to a previously published protocol [137].

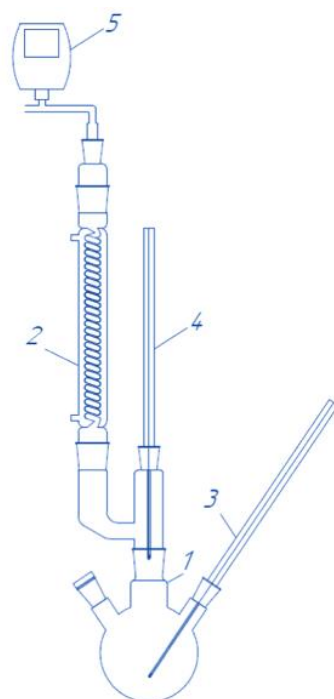
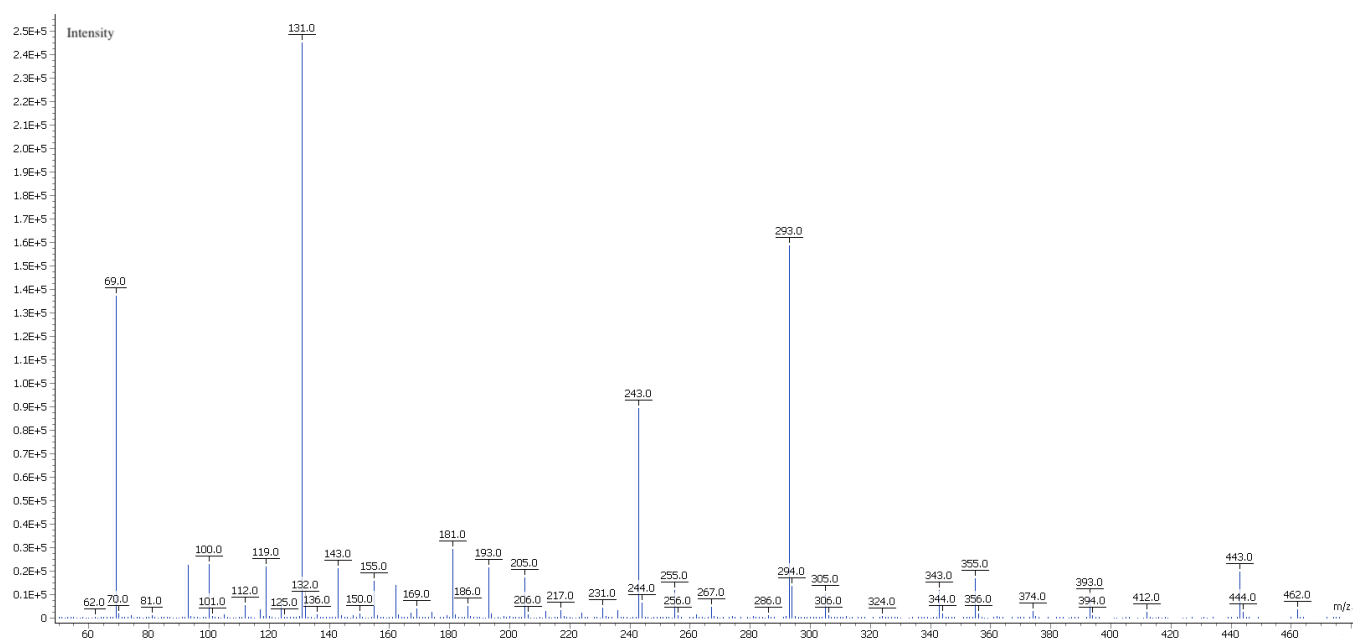


Figure 1. Apparatus for determining saturated vapor pressure: 1—still; 2—backflow condenser; 3 and 4—thermometers; 5—manometer. Reproduced from ref. [130]. Copyright 2023 American Chemical Society.

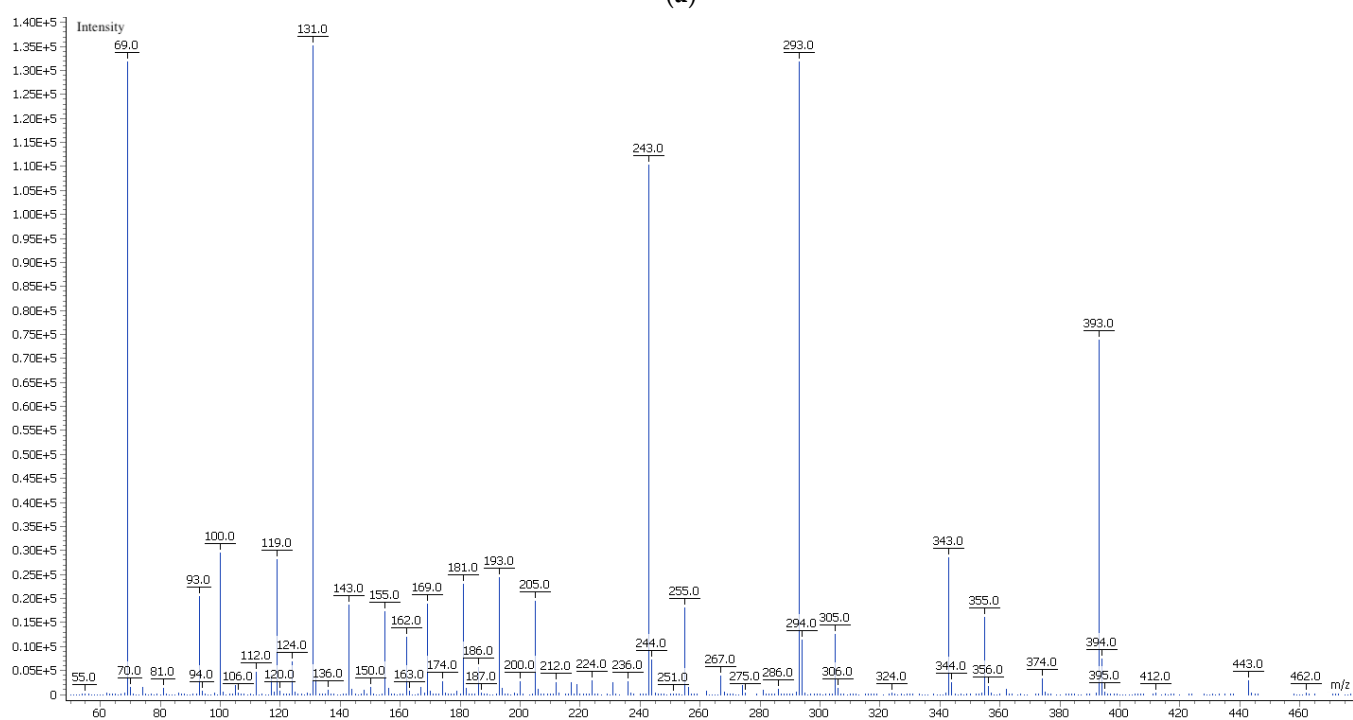
3. Results

3.1. Gas Chromatography–Mass Spectrometry Data

The gas chromatography–mass spectrometry (GC–MS) data for trans-PFD and cis-PFD are shown in Figure 2.



(a)



(b)

Figure 2. GC-MS data: (a) trans-perfluorodecalin; (b) cis-perfluorodecalin.

3.2. NMR and FTIR Spectra

The NMR (^{13}C and ^{19}F) and FTIR spectra for trans-PFD and cis-PFD are shown in Figures 3 and 4, respectively.

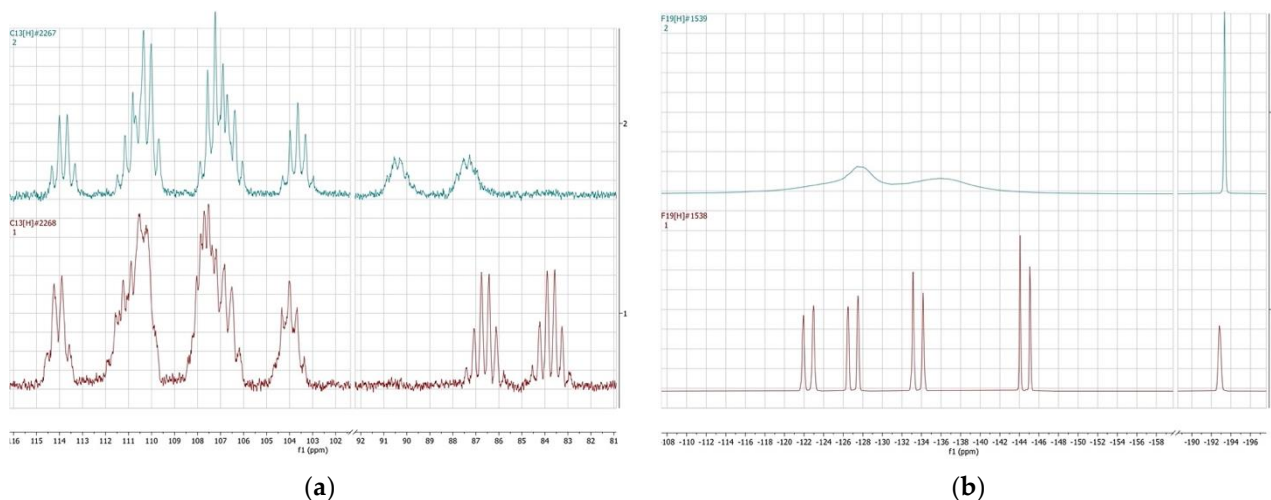
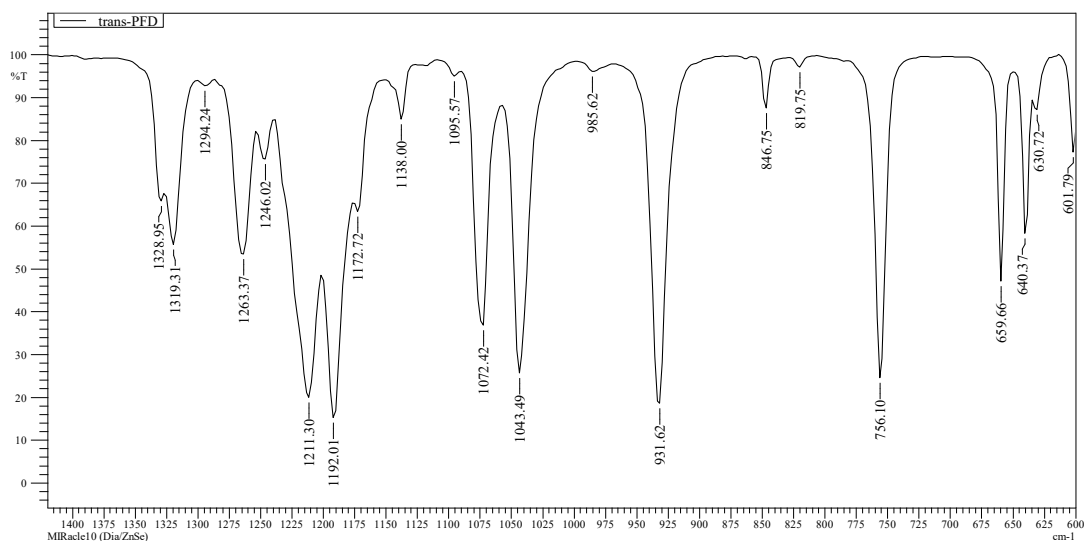
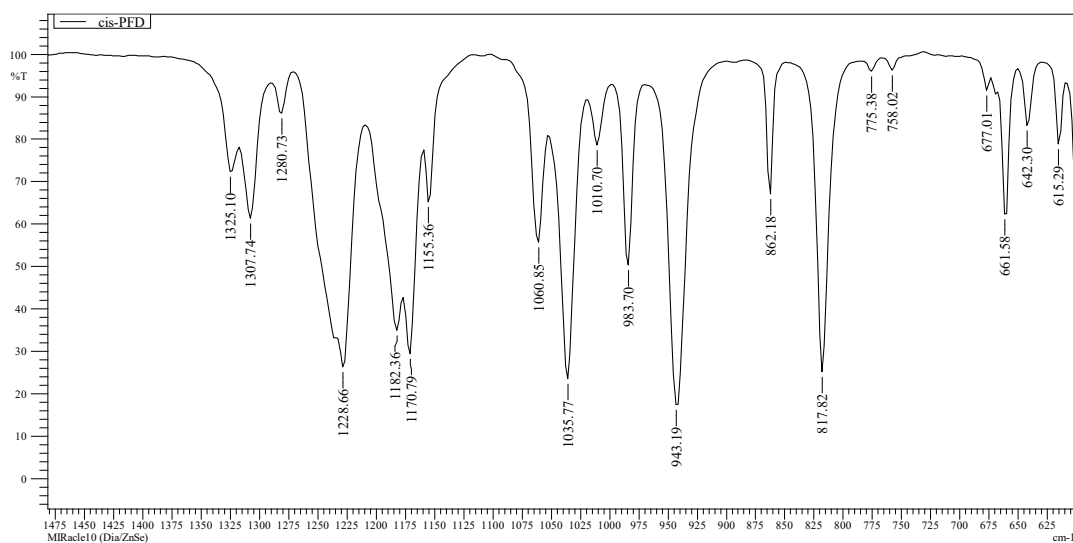


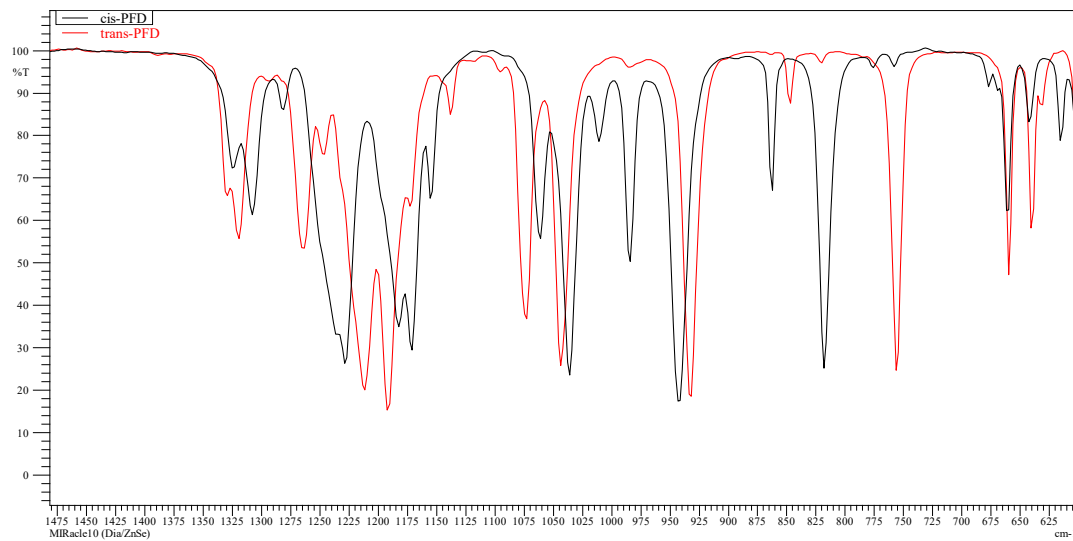
Figure 3. NMR spectrum of trans-perfluorodecalin (red color) and cis-perfluorodecalin (blue color). (a) ^{13}C ; (b) ^{19}F .



(a)



(b)



(c)

Figure 4. FTIR spectra. Fingerprint region of (a) trans-perfluorodecalin, (b) cis-perfluorodecalin, (c) spectra comparison (black—cis-PFD; red—trans-PFD).

3.3. Solid-Liquid Phase Transition

The DSC thermal transition data at a heating/cooling rate $10\text{ }^{\circ}\text{C}\cdot\text{min}^{-1}$ are presented in Figure 5. The data is presented as cooling and heating lines of the weighted samples. All of the heat flow effects are summarized in Table 2.

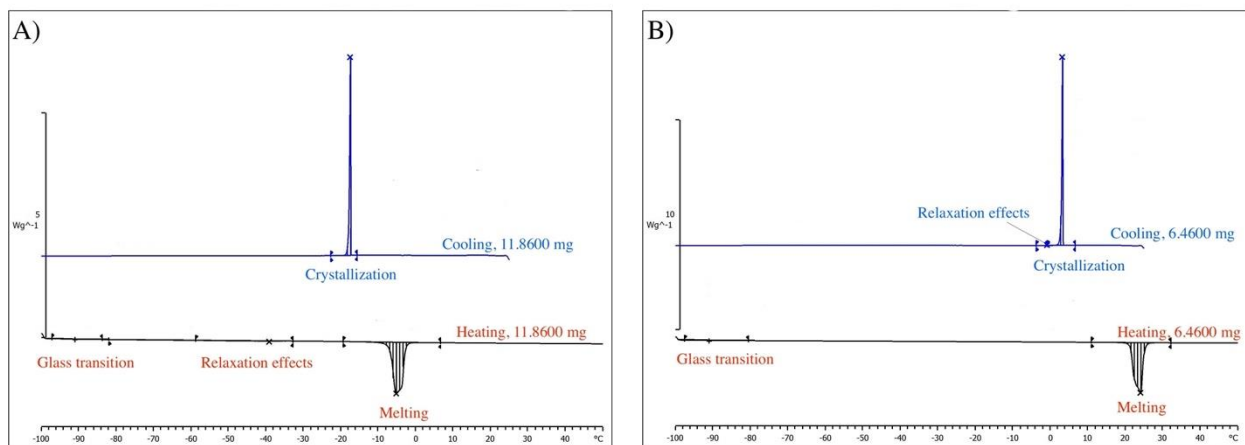


Figure 5. DSC scans. (A) cis-perfluorodecalin; (B) trans-perfluorodecalin.

Table 2. Differential scanning calorimetry data for cis-perfluorodecalin (cis-PFD) and trans-perfluorodecalin (trans-PFD) at sample mass m , temperature T , enthalpy H , heat capacity change ΔC_p , and pressure $P = 98.3$ kPa according to Figure 5 ^a.

| Component | Cis-PFD | | | | Trans-PFD | | | |
|--|-----------------|-------------------------|------------------------|---------|-----------------|------------|-------------------------|---------|
| $m/g \cdot 10^{-3}$ | 11.8600 | | | | 6.4600 | | | |
| type | cooling | heating | | cooling | heating | | cooling | heating |
| Integral/mJ | -244.13 | - | 7.08 | 253.24 | -233.17 | 0.65 | - | 248.15 |
| normalized $H/J \cdot g^{-1}$ | -20.58 | - | 0.60 | 21.35 | -36.09 | 0.10 | - | 38.41 |
| $\Delta C_p/J \cdot g^{-1} \cdot K^{-1}$ | - | 36.930×10^{-3} | - | - | - | - | 49.199×10^{-3} | - |
| onset $T/^\circ C$ | -17.20 | -95.69 | - | -6.99 | 3.48 | -0.74 | -96.57 | 21.22 |
| peak/average point $T/^\circ C$ | -16.24 | -90.94 | -39.11 | -5.44 | 4.67 | -0.90 | -90.93 | 23.55 |
| endset $T/^\circ C$ | -17.65 | -87.60 | - | -2.88 | 3.13 | -1.26 | -85.87 | 24.95 |
| Effect | crystallization | glass transition | solid-solid transition | melting | crystallization | relaxation | glass transition | melting |

^a Standard uncertainties u : $u(m) = 0.01$ g $\cdot 10^{-3}$; $u(T) = 0.25$ °C; $u_r(\text{heat flow}) = 0.05$; $u(P) = 0.3$ kPa.

3.4. Viscosity

Dependences of shear viscosity η on shear rate $\dot{\gamma}$ at different temperatures for trans-PFD and cis-PFD are shown in Figure 6.

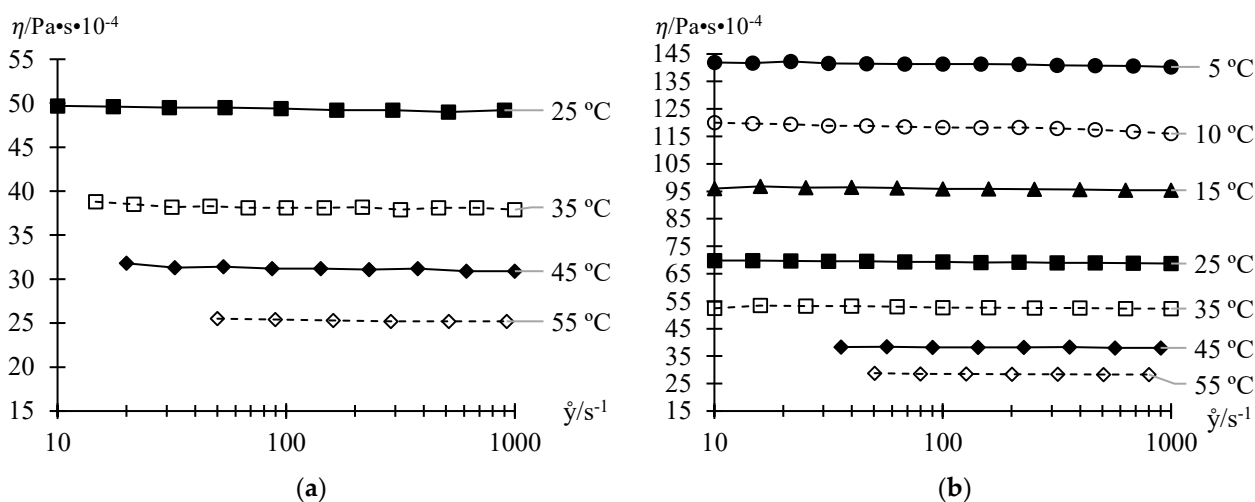


Figure 6. Dependences of shear viscosity η on shear rate $\dot{\gamma}$ at different temperatures T . (a) Trans-perfluorodecalin; (b) cis-perfluorodecalin. Uncertainties: $u(T) = 0.2$ °C; $u_r(\eta) = 0.02$.

Experimental data on the dependences of «zero» shear viscosity on temperature for trans-PFD and cis-PFD are listed in Table 3 and Figure 7.

Table 3. Dependences of «zero» shear viscosity η on temperature T for trans-perfluorodecalin (trans-PFD) and cis-perfluorodecalin (cis-PFD) at pressure $P = 99.3$ kPa ^a.

| $T/^\circ C$ | 5.0 | 10.0 | 15.0 | 25.0 | 35.0 | 45.0 | 55.0 |
|--------------|---------------------------------|-------|------|------|------|------|------|
| Component | $\eta/Pa \cdot s \cdot 10^{-4}$ | | | | | | |
| trans-PFD | - | - | - | 49.4 | 38.2 | 31.2 | 25.3 |
| cis-PFD | 141.3 | 118.3 | 96.0 | 69.3 | 52.7 | 38.2 | 28.5 |

^a Standard uncertainties u : $u(T) = 0.2$ °C; $u_r(\eta) = 0.02$; $u(P) = 0.3$ kPa.

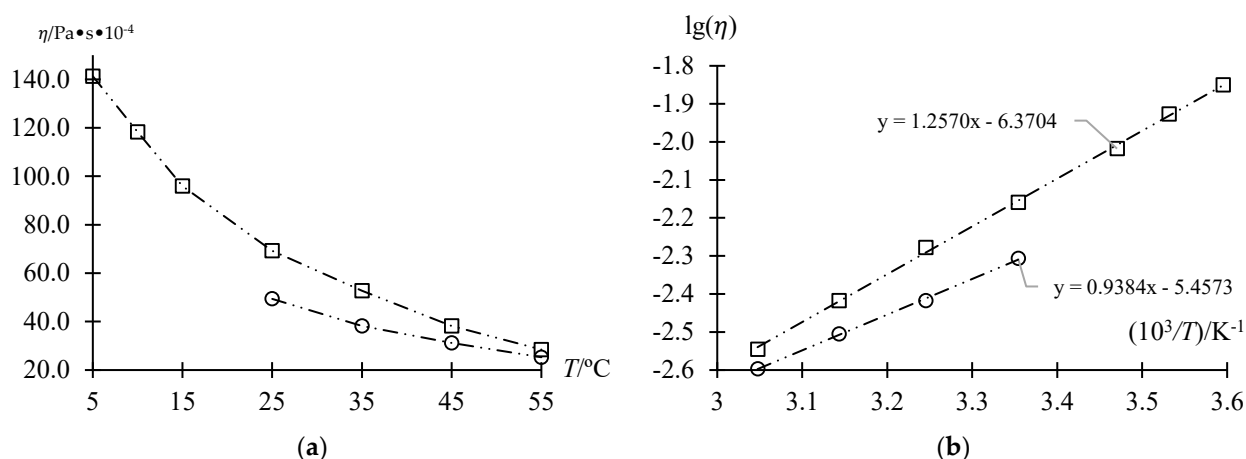


Figure 7. Dependences of «zero» shear viscosity η on temperature T according to Table 3. (a) $\eta = f(T)$; (b) $\lg(\eta) = f(10^3/T)$. Square—cis-perfluorodecalin; circle—trans-perfluorodecalin.

The dependences of the «zero» shear viscosity η of trans-PFD and cis-PFD on temperature T are described by the Arrhenius Equation (1):

$$\lg(\eta) = \lg(\eta_0) - E_a/(2.3 \cdot RT) \quad (1)$$

where η is «zero» shear viscosity, $\text{Pa}\cdot\text{s}$; η_0 is a constant parameter, $\text{Pa}\cdot\text{s}$; E_a represents the apparent activation energy for the viscous flow, $\text{J}\cdot\text{mol}^{-1}$; $R = 8.314$ is the molar gas constant, $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$; T represents temperature, K . The coefficients of the equation are listed in Table 4.

Table 4. Arrhenius Equation (1) coefficients.

| Component | $\eta_0/\text{Pa}\cdot\text{s}\cdot 10^{-6}$ | $E_a/\text{J}\cdot\text{mol}^{-1}$ |
|------------------------|--|------------------------------------|
| trans-perfluorodecalin | 3.489 | -17,944.3 |
| cis-perfluorodecalin | 0.426 | -24,036.6 |

The trans-PFD cooling data up to the crystallization point are shown in Figure 8. The cooling rate was $1^{\circ}\text{C}\cdot\text{min}^{-1}$. The measurements were carried out at a shear rate of $\dot{\gamma} = 30 \text{ s}^{-1}$.

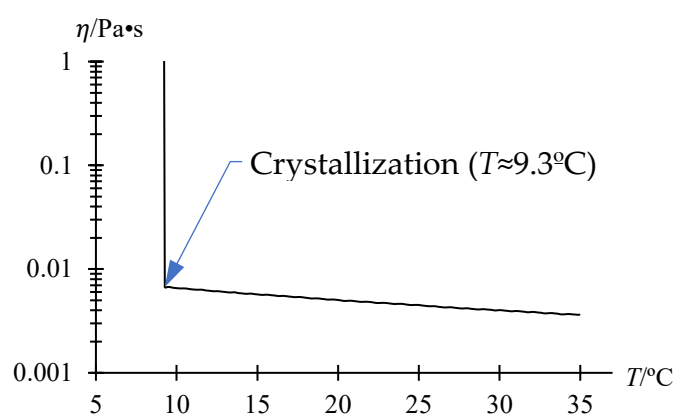


Figure 8. The dependence of shear viscosity of trans-PFD on temperature.

Figure 9 shows summary plots of shear viscosity versus shear rate at 25°C . Additionally, the temperature dependences of viscosity are presented for the MBCN–BCH–trans-PFD–cis-PFD industrial system components of close-boiling isomeric reaction products for the electrochemical fluorination of decalin or naphthalene.

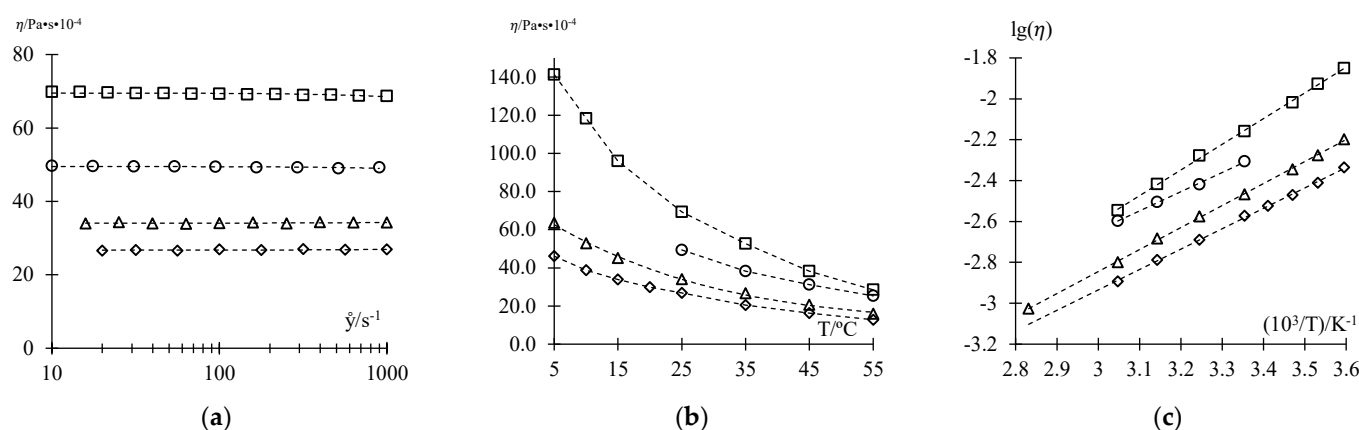


Figure 9. Viscosity data for constituents of the industrial system of the close-boiling isomeric reaction products for the electrochemical fluorination of decalin or naphthalene. (a) $\eta = f(\dot{\gamma})$ at 25 °C; (b) $\eta = f(T)$; (c) $\lg(\eta) = f(1/T)$. Experimental data (Figure 6 and Table 3): circle—trans-perfluorodecalin; square—cis-perfluorodecalin. Literature data [130]: triangular—perfluoro(7-methylbicyclo[4.3.0]nonane); diamond—perfluoro(butylcyclohexane).

3.5. Dependence of the Boiling Temperature on Pressure

Dependence of the saturated vapor pressure, P , of trans-PFD and cis-PFD on temperature T was obtained on the unit depicted in Figure 1; experimental data are listed in Tables 5 and 6.

Table 5. Experimental saturated vapor pressure P data for trans-perfluorodecalin at temperature T ^a.

| $T/^{\circ}\text{C}$ | P/kPa | $T/^{\circ}\text{C}$ | P/kPa | $T/^{\circ}\text{C}$ | P/kPa | $T/^{\circ}\text{C}$ | P/kPa |
|----------------------|----------------|----------------------|----------------|----------------------|----------------|----------------------|----------------|
| 66.0 | 6.3 | 102.0 | 28.2 | 120.4 | 51.6 | 134.3 | 77.7 |
| 74.1 | 9.2 | 105.0 | 31.2 | 122.1 | 54.4 | 136.0 | 81.7 |
| 83.1 | 13.6 | 107.3 | 33.8 | 123.9 | 57.3 | 137.7 | 85.2 |
| 86.6 | 15.6 | 109.4 | 36.1 | 125.2 | 59.8 | 139.2 | 89.1 |
| 89.9 | 17.7 | 112.1 | 39.6 | 126.6 | 62.1 | 140.9 | 93.2 |
| 92.2 | 19.5 | 114.2 | 42.4 | 128.2 | 65.3 | 142.1 | 96.3 |
| 94.1 | 21.0 | 114.7 | 42.8 | 129.9 | 68.4 | 143.5 | 100.1 |
| 96.0 | 22.5 | 116.2 | 45.2 | 131.0 | 71.0 | - | - |
| 97.5 | 23.9 | 118.0 | 47.6 | 132.5 | 73.9 | - | - |
| 99.0 | 25.3 | 118.9 | 48.9 | 133.1 | 75.4 | - | - |

^a Standard uncertainties u are: $u(T) = 0.5$ °C; $u(P) = 0.3$ kPa.

Table 6. Experimental saturated vapor pressure P data for cis-perfluorodecalin at temperature T ^a.

| $T/^{\circ}\text{C}$ | P/kPa | $T/^{\circ}\text{C}$ | P/kPa | $T/^{\circ}\text{C}$ | P/kPa | $T/^{\circ}\text{C}$ | P/kPa |
|----------------------|----------------|----------------------|----------------|----------------------|----------------|----------------------|----------------|
| 78.3 | 10.1 | 105.7 | 30.2 | 118.0 | 45.5 | 137.0 | 81.3 |
| 80.0 | 11.1 | 106.4 | 31.2 | 119.0 | 47.6 | 138.9 | 85.8 |
| 90.9 | 17.2 | 106.8 | 31.4 | 119.7 | 48.5 | 140.0 | 88.8 |
| 93.2 | 19.5 | 107.2 | 32.1 | 120.7 | 49.9 | 141.1 | 91.9 |
| 96.0 | 21.1 | 108.0 | 33.2 | 122.6 | 53.3 | 142.0 | 94.2 |
| 98.6 | 23.4 | 110.0 | 35.2 | 124.6 | 56.6 | 142.7 | 95.7 |
| 100.5 | 25.0 | 112.1 | 38.1 | 127.0 | 60.9 | 143.0 | 96.4 |
| 103.0 | 27.3 | 114.4 | 41.0 | 129.9 | 66.1 | 144.8 | 100.2 |
| 104.8 | 29.2 | 116.1 | 43.4 | 131.9 | 70.0 | - | - |
| 105.0 | 29.6 | 117.0 | 45.1 | 135.2 | 77.6 | - | - |

^a Standard uncertainties u : $u(T) = 0.5$ °C; $u(P) = 0.3$ kPa.

The dependences of the saturated vapor pressure for trans-PFD and cis-PFD on temperature are described by the Antoine Equation (2):

$$\ln P_i = A_i^P + \frac{B_i^P}{T + C_i^P} \quad (2)$$

where P is pressure, kPa; T is temperature, °C; A_i^P , B_i^P , and C_i^P represent coefficients of the Antoine equation. The regressed coefficients of the Antoine equation are presented in Table 7.

Table 7. Antoine Equation (2) coefficients for the temperature range $[T_{\min}, T_{\max}]$.

| Component | A_i^P | B_i^P | C_i^P | $[T_{\min}, T_{\max}]/^{\circ}\text{C}$ |
|------------|---------|------------|---------|---|
| trans-PFD | 12.4765 | -2350.0059 | 155 | [66, 145] |
| cis-PFD | 12.3477 | -2248.9361 | 146 | [78, 144] |
| BCH [130] | 13.5630 | -2900.7119 | 180 | [80, 145] |
| MBCN [130] | 13.5734 | -2916.7343 | 190 | [75, 145] |

The correlation between the data calculated by the Antoine equation (Table 7) and those obtained experimentally (Tables 5 and 6) for saturated vapor pressure versus temperature is presented in the Figure 10; previously reported data [130] for MBCN and BCH are also provided for comparison.

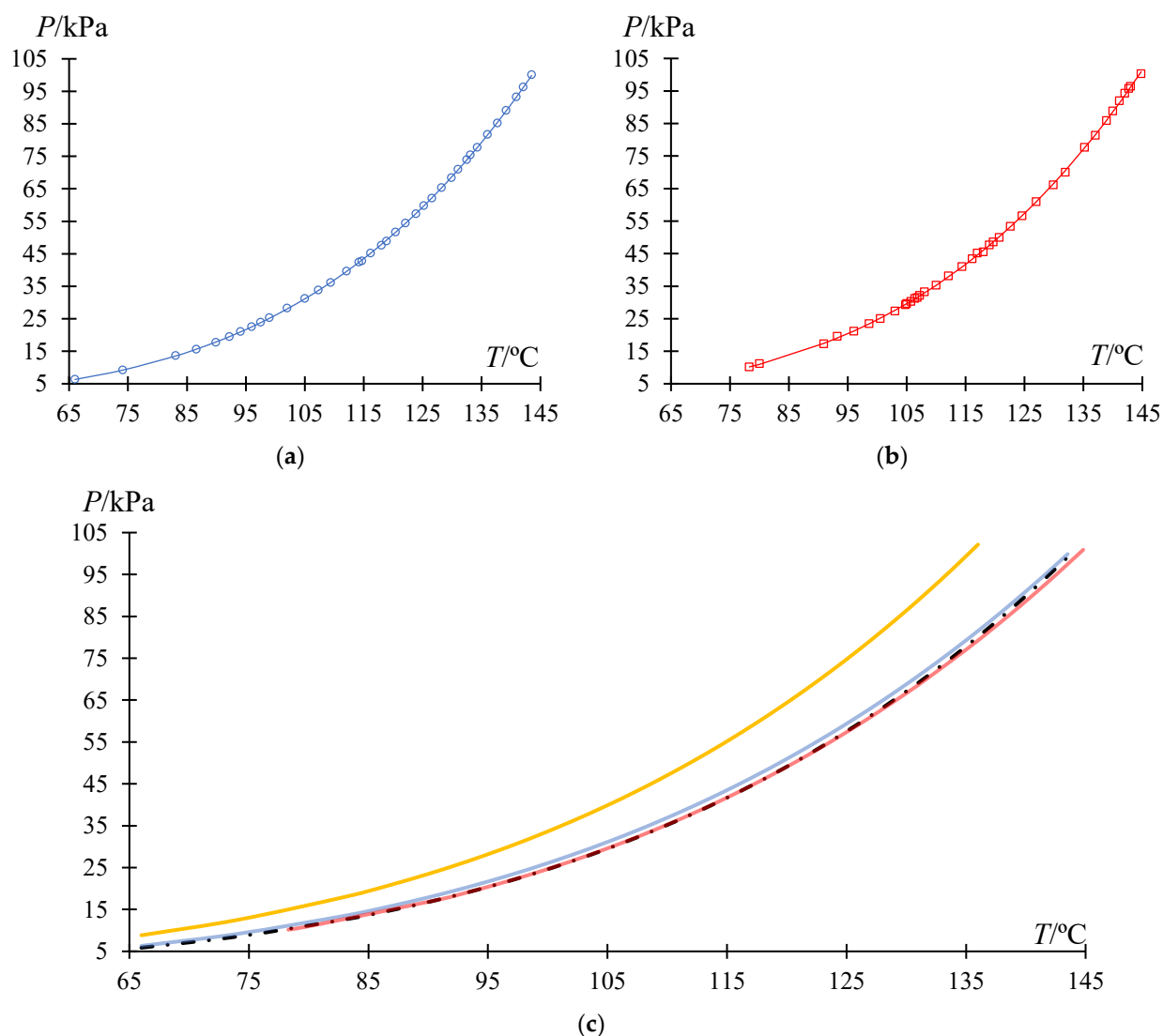


Figure 10. Dependences of the saturated vapor pressure P on temperature T . (a,b) Experimental versus calculated data; (c) isomeric reaction products comparison. Points represent experimental

data (Tables 5 and 6); Lines represent data calculated by the Antoine equation (trans- and cis-PFD: Table 7 data; BCH and MBCN: literature data [130]). Blue: trans-PFD; red: cis-PFD; black: BCH; yellow: MBCN.

3.6. Refractive Index

3.6.1. Pure Substances

Experimental data on the dependences of the refractive index n_D^T on temperature T of trans-PFD and cis-PFD are listed in Tables 8 and 9, respectively.

Table 8. Refractive index n_D^T versus temperature T for trans-perfluorodecalin at pressure $P = 99.0$ kPa ^a.

| $T/^\circ\text{C}$ | n_D | $T/^\circ\text{C}$ | n_D | $T/^\circ\text{C}$ | n_D |
|--------------------|--------|--------------------|--------|--------------------|--------|
| 25.00 | 1.3117 | 37.00 | 1.3073 | 49.00 | 1.3027 |
| 26.00 | 1.3114 | 38.00 | 1.3068 | 50.00 | 1.3023 |
| 27.00 | 1.3110 | 39.00 | 1.3065 | 51.00 | 1.3019 |
| 28.00 | 1.3106 | 40.00 | 1.3061 | 52.00 | 1.3015 |
| 29.00 | 1.3102 | 41.00 | 1.3057 | 53.00 | 1.3011 |
| 30.00 | 1.3099 | 42.00 | 1.3053 | 54.00 | 1.3008 |
| 31.00 | 1.3095 | 43.00 | 1.3050 | 55.00 | 1.3004 |
| 32.00 | 1.3091 | 44.00 | 1.3046 | 56.00 | 1.3000 |
| 33.00 | 1.3088 | 45.00 | 1.3042 | 57.00 | 1.2996 |
| 34.00 | 1.3084 | 46.00 | 1.3038 | 58.00 | 1.2992 |
| 35.00 | 1.3080 | 47.00 | 1.3034 | 59.00 | 1.2988 |
| 36.00 | 1.3076 | 48.00 | 1.3031 | 60.00 | 1.2984 |

^a Standard uncertainties u : $u(T) = 0.05$ °C; $u(n_D) = 0.0001$; $u(P) = 0.3$ kPa.

Table 9. Refractive index n_D^T versus temperature T for cis-perfluorodecalin at pressure $P = 99.2$ kPa ^a.

| $T/^\circ\text{C}$ | n_D | $T/^\circ\text{C}$ | n_D | $T/^\circ\text{C}$ | n_D |
|--------------------|--------|--------------------|--------|--------------------|--------|
| 15.00 | 1.3191 | 31.00 | 1.3131 | 47.00 | 1.3069 |
| 16.00 | 1.3188 | 32.00 | 1.3127 | 48.00 | 1.3065 |
| 17.00 | 1.3184 | 33.00 | 1.3123 | 49.00 | 1.3061 |
| 18.00 | 1.3180 | 34.00 | 1.3119 | 50.00 | 1.3057 |
| 19.00 | 1.3176 | 35.00 | 1.3115 | 51.00 | 1.3053 |
| 20.00 | 1.3173 | 36.00 | 1.3111 | 52.00 | 1.3050 |
| 21.00 | 1.3169 | 37.00 | 1.3108 | 53.00 | 1.3046 |
| 22.00 | 1.3165 | 38.00 | 1.3104 | 54.00 | 1.3042 |
| 23.00 | 1.3161 | 39.00 | 1.3100 | 55.00 | 1.3038 |
| 24.00 | 1.3157 | 40.00 | 1.3096 | 56.00 | 1.3034 |
| 25.00 | 1.3154 | 41.00 | 1.3092 | 57.00 | 1.3030 |
| 26.00 | 1.3150 | 42.00 | 1.3088 | 58.00 | 1.3026 |
| 27.00 | 1.3146 | 43.00 | 1.3085 | 59.00 | 1.3022 |
| 28.00 | 1.3142 | 44.00 | 1.3081 | 60.00 | 1.3018 |
| 29.00 | 1.3138 | 45.00 | 1.3077 | - | - |
| 30.00 | 1.3134 | 46.00 | 1.3073 | - | - |

^a Standard uncertainties u : $u(T) = 0.05$ °C; $u(n_D) = 0.0001$; $u(P) = 0.3$ kPa.

The dependences of the refractive index n_D^T for trans-PFD and cis-PFD on temperature T are described by Equation (3):

$$n_{D_i}^T = A_i^{n_D} + B_i^{n_D} \cdot T/^\circ\text{C} \quad (3)$$

where T is temperature, and °C; $A_i^{n_D}$, and $B_i^{n_D}$ represent coefficients of Equation (3). The coefficients of the equation are listed in Table 10

Table 10. Dimensionless coefficients of Equation (3)—the refractive index n_D^T dependence on temperature T for trans-perfluorodecalin and cis-perfluorodecalin for the temperature range $[T_{\min}, T_{\max}]$.

| Component | $A_i^{n_D}$ | $B_i^{n_D}$ | $[T_{\min}, T_{\max}]/^{\circ}\text{C}$ |
|------------------------|-------------|------------------------|---|
| trans-perfluorodecalin | 1.3213 | -3.80×10^{-4} | [25, 60] |
| cis-perfluorodecalin | 1.3250 | -3.85×10^{-4} | [15, 60] |

The comparison of the experimental (Tables 8 and 9) and calculated (Table 10) dependences for the refractive index of trans-PFD and cis-PFD on temperature are presented in Figure 11.

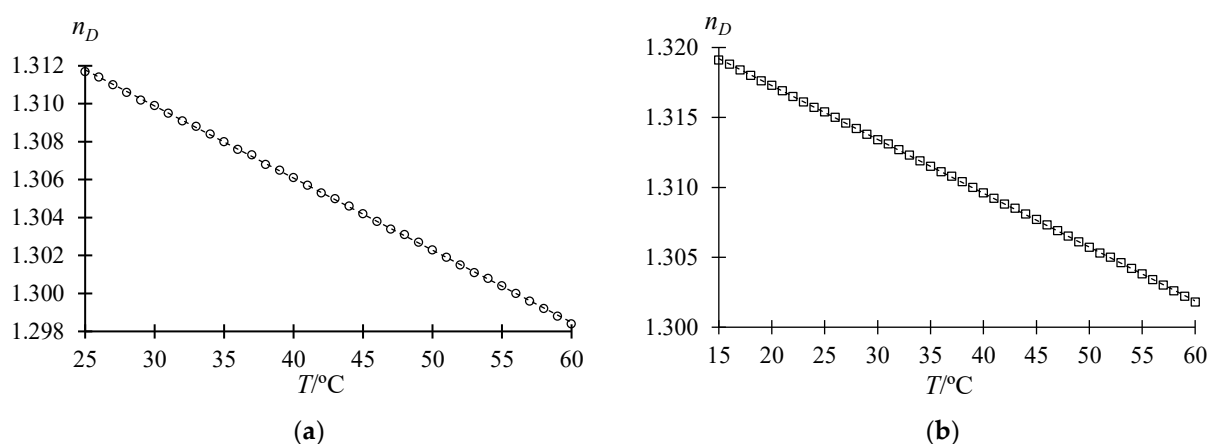


Figure 11. Refractive index n_D^T versus temperature T . (a) trans-perfluorodecalin; (b) cis-perfluorodecalin. Dots: experimental data (Tables 8 and 9); line: calculated by Equation (3) (Table 10).

3.6.2. Binary Systems

Dependences of the refractive index (n_D at 15 and 25 °C) on trans-PFD–cis-PFD, BCH–trans-PFD, and BCH–cis-PFD binary system composition at atmospheric pressure are presented in Table 11 and Figure 12.

Table 11. Dependences of the refractive index n_D^T at temperature T on binary system composition x_i at atmospheric pressure P^a .

| trans-PFD–cis-PFD at $P = 98.2$ kPa | | | BCH–trans-PFD at $P = 100.3$ kPa | | BCH–cis-PFD at $P = 99.4$ kPa | | |
|-------------------------------------|------------|------------|----------------------------------|------------|-------------------------------|------------|------------|
| $x_{\text{trans-PFD}}$ | n_D^{15} | n_D^{25} | x_{BCH} | n_D^{15} | x_{BCH} | n_D^{15} | n_D^{25} |
| 0 | 1.3191 | 1.3154 | 0 | - | 0 | 1.3191 | 1.3154 |
| 0.10198 | 1.3187 | 1.3150 | 0.10688 | 1.3130 | 0.10343 | 1.3163 | 1.3125 |
| 0.19411 | 1.3184 | 1.3146 | 0.19419 | 1.3112 | 0.17164 | 1.3144 | 1.3107 |
| 0.30439 | 1.3180 | 1.3142 | 0.29614 | 1.3091 | 0.28538 | 1.3116 | 1.3079 |
| 0.37857 | 1.3178 | 1.3139 | 0.40515 | 1.3070 | 0.40622 | 1.3089 | 1.3052 |
| 0.49848 | 1.3173 | 1.3135 | 0.49698 | 1.3053 | 0.50224 | 1.3066 | 1.3029 |
| 0.60085 | 1.3169 | 1.3131 | 0.59993 | 1.3034 | 0.60547 | 1.3044 | 1.3007 |
| 0.70172 | 1.3167 | 1.3129 | 0.69763 | 1.3017 | 0.66844 | 1.3027 | 1.2996 |
| 0.80201 | 1.3162 | 1.3125 | 0.80471 | 1.2999 | 0.80202 | 1.3005 | 1.2968 |
| 0.90273 | 1.3159 | 1.3121 | 0.89712 | 1.2979 | 0.88860 | 1.2988 | 1.2952 |
| 1 | - | 1.3117 | 1 | 1.297 | 1 | 1.2970 | - |

^a Standard uncertainties u : $u(T) = 0.05$ °C, $u(n_D) = 0.0001$, $u(P) = 0.3$ kPa, $u(x_i) = 0.00006$.

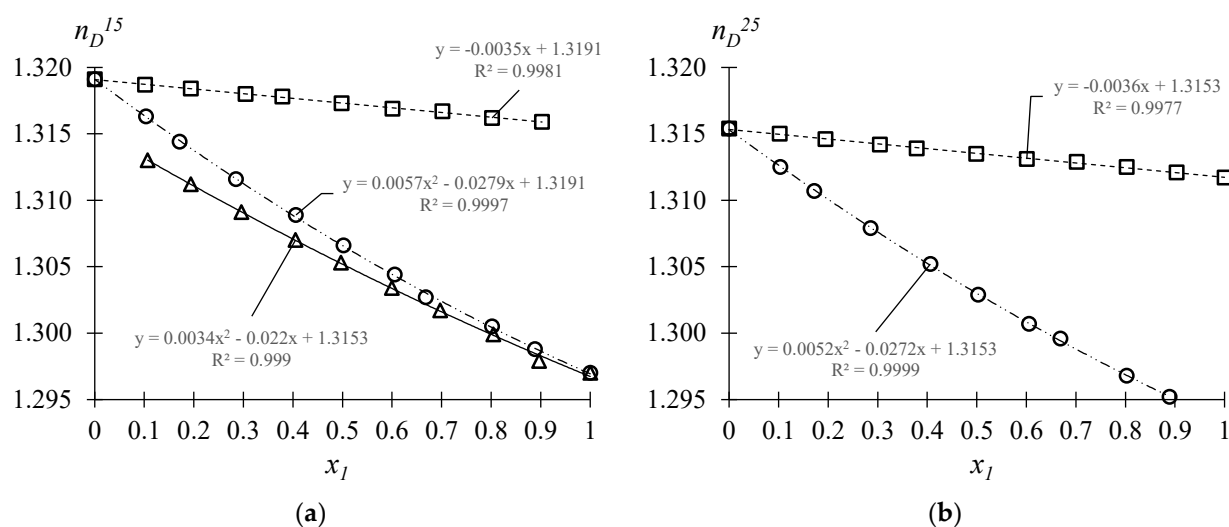


Figure 12. Dependences of the refractive index n_D^T on binary system composition x_i according to the Table 11 data. (a) 15 °C; (b) 25 °C. Square trans-PFD (1)–cis-PFD (2); circle BCH (1)–cis-PFD (2); triangular BCH (1)–trans-PFD (2).

The equation for the dependence of the refractive index on the compositions of the trans-PFD–cis-PFD, BCH–trans-PFD, and BCH–cis-PFD binary systems was generated based on the data shown in Figure 12; the coefficients for Equation (4) are listed in Table 12:

$$n_D = a_0^{n_D} + a_1^{n_D} x_1 + a_2^{n_D} x_1^2 \quad (4)$$

where x_1 is the composition, mole fraction; $a_0^{n_D}$, $a_1^{n_D}$, and $a_2^{n_D}$ are coefficients of Equation (4).

Table 12. Dimensionless coefficients of Equation (4)—the refractive index n_D^T dependence on binary systems composition x_i at temperature T .

| System | trans-PFD (1)–cis-PFD (2) | | BCH (1)–trans-PFD (2) | | BCH (1)–cis-PFD (2) | |
|---------------|---------------------------|---------|-----------------------|---------|---------------------|---------|
| $T/\text{°C}$ | 15 | 25 | 15 | 25 | 15 | 25 |
| $a_0^{n_D}$ | 1.3191 | 1.3153 | 1.3153 | 1.3191 | 1.3191 | 1.3153 |
| $a_1^{n_D}$ | −0.0035 | −0.0036 | −0.0220 | −0.0279 | −0.0279 | −0.0272 |
| $a_2^{n_D}$ | 0 | 0 | 0.0034 | 0.0057 | 0.0057 | 0.0052 |

3.6.3. Ternary System

Dependence of the refractive index (n_D at 15 and 25 °C) on the BCH–trans-PFD–cis-PFD ternary system composition at atmospheric pressure is presented in Table 13 and Figure 13.

Table 13. Dependences of the refractive index n_D^T at temperature T on BCH (1)–trans-PFD (2)–cis-PFD (3) ternary system composition x_i at pressure $P = 99.1\text{ kPa}$ ^a.

| x_1 | x_2 | x_3 | n_D^{15} | n_D^{25} |
|---------|---------|---------|------------|------------|
| 0.57402 | 0.21988 | 0.20610 | 1.3046 | 1.3003 |
| 0.17937 | 0.63244 | 0.18819 | 1.3121 | 1.3085 |
| 0.17479 | 0.19519 | 0.63002 | 1.3137 | 1.3099 |
| 0.18870 | 0.39863 | 0.41267 | 1.3128 | 1.3091 |
| 0.37885 | 0.22255 | 0.39860 | 1.3087 | 1.3050 |
| 0.36974 | 0.40875 | 0.22151 | 1.3083 | 1.3046 |

^a Standard uncertainties u : $u(T) = 0.05\text{ °C}$, $u(n_D) = 0.0001$, $u(P) = 0.3\text{ kPa}$, $u(x_i) = 0.00005$.

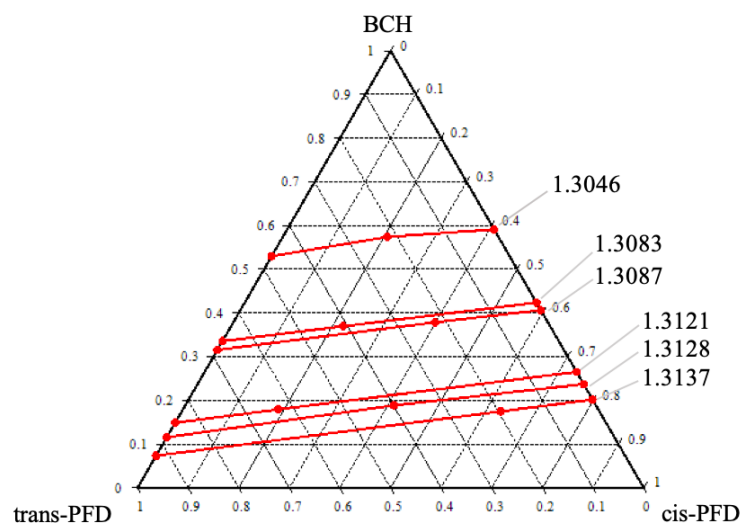


Figure 13. Dependence of the isoline of refractive index on ternary system composition according to the data from Tables 12 and 13 at 15 °C.

3.7. Density and Liquid Molar Volume

3.7.1. Pure Substances

Experimental data on the dependences of the density ρ_i and liquid molar volume V_{M_i} on the temperature of trans-PFD and cis-PFD are presented in Tables 14 and 15, respectively.

Table 14. Density ρ and liquid molar volume V_M versus temperature T for trans-perfluorodecalin at pressure $P = 99.0$ kPa ^a.

| $T/^\circ\text{C}$ | $\rho/\text{g}\cdot\text{cm}^{-3}$ | $V_M/\text{cm}^3\cdot\text{mol}^{-1}$ | $T/^\circ\text{C}$ | $\rho/\text{g}\cdot\text{cm}^{-3}$ | $V_M/\text{cm}^3\cdot\text{mol}^{-1}$ | $T/^\circ\text{C}$ | $\rho/\text{g}\cdot\text{cm}^{-3}$ | $V_M/\text{cm}^3\cdot\text{mol}^{-1}$ |
|--------------------|------------------------------------|---------------------------------------|--------------------|------------------------------------|---------------------------------------|--------------------|------------------------------------|---------------------------------------|
| 25.00 | 1.92344 | 240.236 | 37.00 | 1.89637 | 243.666 | 49.00 | 1.86915 | 247.214 |
| 26.00 | 1.92116 | 240.521 | 38.00 | 1.89411 | 243.956 | 50.00 | 1.86687 | 247.516 |
| 27.00 | 1.91890 | 240.805 | 39.00 | 1.89186 | 244.246 | 51.00 | 1.86458 | 247.820 |
| 28.00 | 1.91663 | 241.090 | 40.00 | 1.88960 | 244.539 | 52.00 | 1.86230 | 248.123 |
| 29.00 | 1.91438 | 241.373 | 41.00 | 1.88734 | 244.831 | 53.00 | 1.86002 | 248.427 |
| 30.00 | 1.91213 | 241.657 | 42.00 | 1.88507 | 245.126 | 54.00 | 1.85771 | 248.736 |
| 31.00 | 1.90987 | 241.943 | 43.00 | 1.88280 | 245.422 | 55.00 | 1.85542 | 249.043 |
| 32.00 | 1.90763 | 242.227 | 44.00 | 1.88053 | 245.718 | 56.00 | 1.85312 | 249.352 |
| 33.00 | 1.90537 | 242.515 | 45.00 | 1.87826 | 246.015 | 57.00 | 1.85083 | 249.661 |
| 34.00 | 1.90312 | 242.801 | 46.00 | 1.87599 | 246.313 | 58.00 | 1.84850 | 249.976 |
| 35.00 | 1.90087 | 243.089 | 47.00 | 1.87371 | 246.612 | 59.00 | 1.84620 | 250.287 |
| 36.00 | 1.89862 | 243.377 | 48.00 | 1.87143 | 246.913 | 60.00 | 1.84389 | 250.601 |

^a Standard uncertainties u : $u(T) = 0.05$ °C; $u(\rho) = 0.0001$ g·cm⁻³; $u(P) = 0.3$ kPa.

Table 15. Density ρ and liquid molar volume V_M versus temperature T for cis-perfluorodecalin at pressure $P = 99.2$ kPa ^a.

| $T/^\circ\text{C}$ | $\rho/\text{g}\cdot\text{cm}^{-3}$ | $V_M/\text{cm}^3\cdot\text{mol}^{-1}$ | $T/^\circ\text{C}$ | $\rho/\text{g}\cdot\text{cm}^{-3}$ | $V_M/\text{cm}^3\cdot\text{mol}^{-1}$ | $T/^\circ\text{C}$ | $\rho/\text{g}\cdot\text{cm}^{-3}$ | $V_M/\text{cm}^3\cdot\text{mol}^{-1}$ |
|--------------------|------------------------------------|---------------------------------------|--------------------|------------------------------------|---------------------------------------|--------------------|------------------------------------|---------------------------------------|
| 15.00 | 1.96878 | 234.704 | 31.00 | 1.93225 | 239.141 | 47.00 | 1.89598 | 243.716 |
| 16.00 | 1.96653 | 234.972 | 32.00 | 1.93025 | 239.389 | 48.00 | 1.89354 | 244.030 |
| 17.00 | 1.96427 | 235.243 | 33.00 | 1.92797 | 239.672 | 49.00 | 1.89133 | 244.315 |
| 18.00 | 1.96201 | 235.514 | 34.00 | 1.92569 | 239.956 | 50.00 | 1.88908 | 244.606 |
| 19.00 | 1.95973 | 235.788 | 35.00 | 1.92341 | 240.240 | 51.00 | 1.88674 | 244.909 |
| 20.00 | 1.95746 | 236.061 | 36.00 | 1.92113 | 240.525 | 52.00 | 1.88442 | 245.211 |

| | | | | | | | | |
|-------|---------|---------|-------|---------|---------|-------|---------|---------|
| 21.00 | 1.95520 | 236.334 | 37.00 | 1.91885 | 240.811 | 53.00 | 1.88209 | 245.514 |
| 22.00 | 1.95293 | 236.609 | 38.00 | 1.91656 | 241.099 | 54.00 | 1.87975 | 245.820 |
| 23.00 | 1.95066 | 236.884 | 39.00 | 1.91427 | 241.387 | 55.00 | 1.87743 | 246.124 |
| 24.00 | 1.94840 | 237.159 | 40.00 | 1.91198 | 241.676 | 56.00 | 1.87510 | 246.430 |
| 25.00 | 1.94613 | 237.435 | 41.00 | 1.90968 | 241.967 | 57.00 | 1.87276 | 246.737 |
| 26.00 | 1.94387 | 237.711 | 42.00 | 1.90738 | 242.259 | 58.00 | 1.87043 | 247.045 |
| 27.00 | 1.94160 | 237.989 | 43.00 | 1.90509 | 242.550 | 59.00 | 1.86810 | 247.353 |
| 28.00 | 1.93933 | 238.268 | 44.00 | 1.90278 | 242.845 | 60.00 | 1.86576 | 247.663 |
| 29.00 | 1.93707 | 238.546 | 45.00 | 1.90064 | 243.118 | - | - | - |
| 30.00 | 1.93480 | 238.826 | 46.00 | 1.89829 | 243.419 | - | - | - |

^a Standard uncertainties u : $u(T) = 0.05$ °C; $u(\rho) = 0.0001$ g·cm⁻³; $u(P) = 0.3$ kPa.

Liquid molar volume V_{M_i} presented in Tables 14 and 15 was calculated according to Equation (5):

$$V_{M_i} = \frac{M_i}{\rho_i} \quad (5)$$

where M_i is molecular weight, g·mol⁻¹; ρ_i is density, g·cm⁻³.

The dependences of the density ρ_i of trans-PFD and cis-PFD on temperature T are described by Equation (6):

$$\rho_i(\text{g} \cdot \text{cm}^{-3}) = A_i^\rho + B_i^\rho \cdot T/^\circ\text{C} \quad (6)$$

where T is temperature, °C; A_i^ρ and B_i^ρ are coefficients of Equation (6); the coefficients are listed in Table 16

Table 16. Coefficients of Equation (6)—the density (ρ) dependence on temperature (T) for trans-perfluorodecalin and cis-perfluorodecalin.

| Component | A_i^ρ | B_i^ρ | $[T_{\min}, T_{\max}]/^\circ\text{C}$ |
|------------------------|------------|------------|---------------------------------------|
| Trans-perfluorodecalin | 1.98029 | -0.00227 | [25, 60] |
| Cis-perfluorodecalin | 2.00330 | -0.00229 | [15, 60] |

The comparison of the calculated (Table 16) and experimental (Tables 14 and 15) dependences for the density and liquid molar volume of trans-PFD and cis-PFD on temperature are presented in Figure 14.

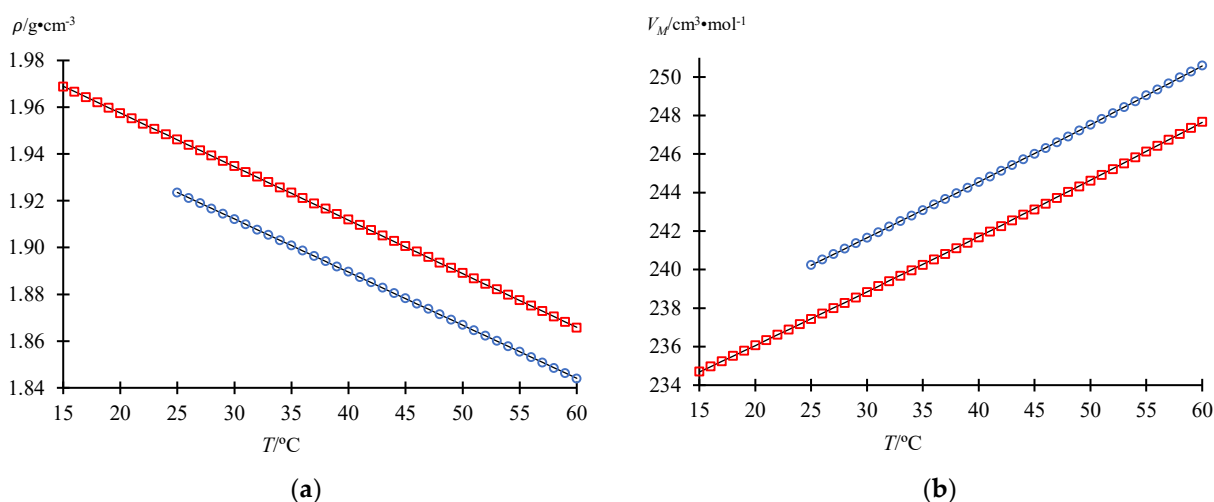


Figure 14. Experimental values of density ρ (a) and liquid molar volume V_M (b) versus temperature T . blue dots: trans-perfluorodecalin (Table 14), red dots: cis-perfluorodecalin (Table 15), lines: data calculated by Equations (5) and (6) (Table 16).

3.7.2. Binary Systems

Dependences of density on the composition of BCH–cis-PFD, BCH–trans-PFD, and trans-PFD–cis-PFD systems at different temperatures are presented in Tables 17–19, respectively.

Table 17. Dependences of density ρ on perfluoro(butylcyclohexane) (1)–cis-perfluorodecalin (2) system composition x_i at temperature T and pressure P ^a.

| x_1 | P/kPa | $T/^\circ\text{C}$ | | | | | | | | | |
|---------|----------------|------------------------------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| | | 15 | 20 | 25 | 30 | 35 | 40 | 45 | 50 | 55 | 60 |
| | | $\rho/\text{g}\cdot\text{cm}^{-3}$ | | | | | | | | | |
| 0 | 99.2 | 1.96878 | 1.95746 | 1.94613 | 1.93480 | 1.92341 | 1.91198 | 1.90048 | 1.88908 | 1.87743 | 1.86576 |
| 0.10343 | | 1.95773 | 1.94661 | 1.93538 | 1.92409 | 1.91274 | 1.90134 | 1.88990 | 1.87837 | 1.86681 | 1.85514 |
| 0.17164 | 98.8 | 1.95040 | 1.93938 | 1.92823 | 1.91699 | 1.90568 | 1.89431 | 1.88287 | 1.87133 | 1.85977 | 1.84813 |
| 0.28538 | | 1.93986 | 1.92883 | 1.91769 | 1.90648 | 1.89518 | 1.88382 | 1.87239 | 1.86088 | 1.84931 | 1.83769 |
| 0.31744 | 100.5 | 1.93729 | 1.92620 | 1.91502 | 1.90376 | 1.89245 | 1.88103 | 1.86963 | 1.85817 | 1.84662 | 1.83500 |
| 0.35826 | | 1.93361 | 1.92262 | 1.91148 | 1.90026 | 1.88896 | 1.87761 | 1.86616 | 1.85466 | 1.84311 | 1.83149 |
| 0.37933 | 98.8 | 1.93190 | 1.92084 | 1.90966 | 1.89842 | 1.88711 | 1.87577 | 1.86434 | 1.85285 | 1.84132 | 1.82971 |
| 0.39919 | | 1.92998 | 1.91897 | 1.90783 | 1.89661 | 1.88532 | 1.87394 | 1.86252 | 1.85100 | 1.83945 | 1.82783 |
| 0.44022 | 100.5 | 1.92669 | 1.91568 | 1.90455 | 1.89334 | 1.88204 | 1.87067 | 1.85925 | 1.84772 | 1.83616 | 1.82452 |
| 0.50224 | 98.9 | 1.92200 | 1.91097 | 1.89981 | 1.88859 | 1.87728 | 1.86590 | 1.85445 | 1.84290 | 1.83134 | 1.81967 |
| 0.60547 | | 1.91379 | 1.90281 | 1.89167 | 1.88044 | 1.86912 | 1.85772 | 1.84626 | 1.83471 | 1.82309 | 1.81141 |
| 0.69350 | | 1.90737 | 1.89625 | 1.88502 | 1.87373 | 1.86236 | 1.85095 | 1.83944 | 1.82786 | 1.81625 | 1.80453 |
| 0.80202 | 100.3 | 1.89986 | 1.88879 | 1.87760 | 1.86631 | 1.85493 | 1.84345 | 1.83192 | 1.82027 | 1.80859 | 1.79682 |
| 0.88860 | | 1.89420 | 1.88309 | 1.87186 | 1.86052 | 1.84911 | 1.83760 | 1.82603 | 1.81436 | 1.80264 | 1.79081 |
| 1 | 99.3 | 1.88829 | 1.87697 | 1.86563 | 1.85429 | 1.84283 | 1.83130 | 1.81969 | 1.80795 | 1.79625 | 1.78436 |

^a Standard uncertainties u : $u(T) = 0.05$ °C; $u(x_i) = 0.00005$; $u(\rho) = 0.0001$ g·cm⁻³; $u(P) = 0.3$ kPa.

Table 18. Dependences of the density ρ on perfluoro(butylcyclohexane) (1)–trans-perfluorodecalin (2) system composition x_i at temperature T and pressure P ^a.

| x_1 | P/kPa | $T/^\circ\text{C}$ | | | | | | | | |
|---------|----------------|------------------------------------|---------|---------|---------|---------|---------|---------|---------|--|
| | | 25 | 30 | 35 | 40 | 45 | 50 | 55 | 60 | |
| | | $\rho/\text{g}\cdot\text{cm}^{-3}$ | | | | | | | | |
| 0 | 98.1 | 1.92344 | 1.91213 | 1.90087 | 1.88960 | 1.87826 | 1.86687 | 1.85542 | 1.84389 | |
| 0.10688 | | 1.91545 | 1.90436 | 1.89319 | 1.88195 | 1.87063 | 1.85923 | 1.84778 | 1.83623 | |
| 0.19419 | 100.7 | 1.90908 | 1.89804 | 1.88689 | 1.87565 | 1.86434 | 1.85294 | 1.84149 | 1.82996 | |
| 0.29614 | | 1.90250 | 1.89142 | 1.88025 | 1.86900 | 1.85767 | 1.84624 | 1.83478 | 1.82322 | |
| 0.40516 | | 1.89601 | 1.88487 | 1.87363 | 1.86233 | 1.85096 | 1.83953 | 1.82801 | 1.81643 | |
| 0.49698 | 99.3 | 1.89052 | 1.87939 | 1.86815 | 1.85684 | 1.84545 | 1.83396 | 1.82240 | 1.81078 | |
| 0.59993 | | 1.88470 | 1.87354 | 1.86227 | 1.85091 | 1.83947 | 1.82794 | 1.81635 | 1.80468 | |
| 0.69763 | | 1.87961 | 1.86836 | 1.85703 | 1.84562 | 1.83415 | 1.82258 | 1.81093 | 1.79920 | |
| 0.80471 | 99.7 | 1.87398 | 1.86272 | 1.85135 | 1.83990 | 1.82837 | 1.81675 | 1.80507 | 1.79330 | |
| 0.89712 | | 1.86994 | 1.85859 | 1.84715 | 1.83560 | 1.82404 | 1.81237 | 1.80064 | 1.78882 | |
| 1 | 99.3 | 1.86563 | 1.85429 | 1.84283 | 1.83130 | 1.81969 | 1.80795 | 1.79625 | 1.78436 | |

^a Standard uncertainties u : $u(T) = 0.05$ °C; $u(x_i) = 0.00006$; $u(\rho) = 0.0001$ g·cm⁻³; $u(P) = 0.3$ kPa.

Table 19. Dependences of the density ρ on trans-perfluorodecalin (1)–cis-perfluorodecalin (2) system composition x_i at temperature T and pressure P ^a.

| x_1 | P/kPa | $T/^\circ\text{C}$ | | | | | | | |
|---------|----------------|------------------------------------|---------|---------|---------|---------|---------|---------|---------|
| | | 25 | 30 | 35 | 40 | 45 | 50 | 55 | 60 |
| | | $\rho/\text{g}\cdot\text{cm}^{-3}$ | | | | | | | |
| 0 | 99.2 | 1.94613 | 1.93480 | 1.92341 | 1.91198 | 1.90079 | 1.88908 | 1.87743 | 1.86576 |
| 0.10198 | | 1.94389 | 1.93263 | 1.92128 | 1.90985 | 1.89839 | 1.88684 | 1.87527 | 1.86360 |
| 0.19411 | 100.9 | 1.94178 | 1.93058 | 1.91926 | 1.90787 | 1.89640 | 1.88487 | 1.87330 | 1.86165 |
| 0.30439 | | 1.93933 | 1.92811 | 1.91681 | 1.90544 | 1.89397 | 1.88244 | 1.87085 | 1.85919 |
| 0.41417 | 100.0 | 1.93671 | 1.92547 | 1.91416 | 1.90279 | 1.89136 | 1.87988 | 1.86832 | 1.85670 |
| 0.49848 | | 1.93455 | 1.92338 | 1.91210 | 1.90076 | 1.88933 | 1.87785 | 1.86631 | 1.85470 |
| 0.60085 | 100.8 | 1.93220 | 1.92104 | 1.90978 | 1.89845 | 1.88704 | 1.87557 | 1.86404 | 1.85246 |
| 0.70172 | 99.7 | 1.92985 | 1.91870 | 1.90745 | 1.89617 | 1.88479 | 1.87335 | 1.86184 | 1.85029 |
| 0.80539 | 100.1 | 1.92740 | 1.91631 | 1.90510 | 1.89382 | 1.88247 | 1.87106 | 1.85956 | 1.84799 |
| 0.90273 | 99.7 | 1.92528 | 1.91420 | 1.90300 | 1.89173 | 1.88039 | 1.86895 | 1.85746 | 1.84592 |
| 1 | 98.1 | 1.92344 | 1.91213 | 1.90087 | 1.88960 | 1.87826 | 1.86687 | 1.85542 | 1.84389 |

^a Standard uncertainties u : $u(T) = 0.05$ °C; $u(x_i) = 0.00006$; $u(\rho) = 0.0001$ g·cm⁻³; $u(P) = 0.3$ kPa.

The liquid molar volume V_M of the BCH–cis-PFD, BCH–trans-PFD, and trans-PFD–cis-PFD systems was calculated according to Equation (7) and is presented in Tables 20–22, respectively. Additionally, the excess molar volume V^E of the BCH–cis-PFD, BCH–trans-PFD, and trans-PFD–cis-PFD systems was calculated according to Equation (8) and is presented in Tables 23–25, respectively. The V_M and V^E data (Tables 20–25) provide the maximum standard uncertainties u of the values; standard uncertainties u for each experimental point are provided in Appendix A (Tables A1–A6, respectively).

$$V_M = \frac{\sum_{i=1}^i M_i x_i}{\rho_{mixture}} \quad (7)$$

$$V^E = \frac{x_i M_i + x_j M_j}{\rho_{mixture}} - \left(x_i \frac{M_i}{\rho_i} + x_j \frac{M_j}{\rho_j} \right) \quad (8)$$

where M_i is the molecular weight, g·mol⁻¹; $\rho_{mixture}$ is the mixture density at composition x_i , g·cm⁻³.

Table 20. Dependences of the liquid molar volume V_M on perfluoro(butylcyclohexane) (1)–cis-perfluorodecalin (2) system composition x_i at temperature T ^a.

| x_1 | $T/^\circ\text{C}$ | | | | | | | | | |
|---------|--|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| | 15 | 20 | 25 | 30 | 35 | 40 | 45 | 50 | 55 | 60 |
| | $V_M/\text{cm}^{-3}\cdot\text{mol}^{-1}$ | | | | | | | | | |
| 0 | 234.704 | 236.061 | 237.435 | 238.826 | 240.240 | 241.676 | 243.139 | 244.606 | 246.124 | 247.663 |
| 0.10343 | 238.036 | 239.395 | 240.784 | 242.197 | 243.634 | 245.095 | 246.579 | 248.092 | 249.629 | 251.199 |
| 0.17164 | 240.259 | 241.624 | 243.021 | 244.446 | 245.897 | 247.373 | 248.876 | 250.410 | 251.967 | 253.554 |
| 0.28538 | 243.792 | 245.186 | 246.610 | 248.060 | 249.539 | 251.044 | 252.576 | 254.139 | 255.729 | 257.346 |
| 0.31744 | 244.744 | 246.153 | 247.590 | 249.054 | 250.543 | 252.064 | 253.601 | 255.165 | 256.761 | 258.387 |
| 0.35826 | 246.012 | 247.418 | 248.860 | 250.329 | 251.827 | 253.349 | 254.903 | 256.484 | 258.091 | 259.729 |
| 0.37933 | 246.644 | 248.064 | 249.516 | 250.993 | 252.498 | 254.024 | 255.581 | 257.166 | 258.777 | 260.419 |
| 0.39919 | 247.280 | 248.699 | 250.151 | 251.631 | 253.138 | 254.675 | 256.236 | 257.831 | 259.450 | 261.099 |
| 0.44022 | 248.511 | 249.939 | 251.400 | 252.889 | 254.407 | 255.953 | 257.525 | 259.132 | 260.764 | 262.427 |
| 0.50224 | 250.343 | 251.788 | 253.267 | 254.772 | 256.307 | 257.870 | 259.462 | 261.089 | 262.737 | 264.422 |
| 0.60547 | 253.467 | 254.929 | 256.430 | 257.962 | 259.524 | 261.117 | 262.738 | 264.392 | 266.077 | 267.792 |

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| 0.69350 | 256.073 | 257.575 | 259.109 | 260.670 | 262.262 | 263.879 | 265.530 | 267.212 | 268.920 | 270.667 |
| 0.80202 | 259.255 | 260.775 | 262.329 | 263.916 | 265.535 | 267.189 | 268.870 | 270.591 | 272.339 | 274.122 |
| 0.88860 | 261.766 | 263.311 | 264.890 | 266.505 | 268.149 | 269.829 | 271.539 | 273.285 | 275.062 | 276.879 |
| 1 | 264.827 | 266.424 | 268.044 | 269.683 | 271.360 | 273.068 | 274.811 | 276.595 | 278.397 | 280.252 |

^a Standard uncertainties u : $u(T) = 0.05$ °C; $u(x_i) = 0.00005$; $u(V_M) = 0.025$ cm³·mol⁻¹.

Table 21. Dependences of the liquid molar volume V_M on perfluoro(butylcyclohexane) (1)–trans-perfluorodecalin (2) system composition x_i at temperature T ^a.

| x_1 | $T/^\circ\text{C}$ | | | | | | | | |
|---------|---------------------------------------|---------|---------|---------|---------|---------|---------|---------|--|
| | 25 | 30 | 35 | 40 | 45 | 50 | 55 | 60 | |
| | $V_M/\text{cm}^3\cdot\text{mol}^{-1}$ | | | | | | | | |
| 0 | 240.236 | 241.657 | 243.089 | 244.539 | 246.015 | 247.516 | 249.043 | 250.601 | |
| 0.10688 | 243.358 | 244.775 | 246.220 | 247.690 | 249.189 | 250.717 | 252.270 | 253.857 | |
| 0.19419 | 245.908 | 247.338 | 248.799 | 250.290 | 251.809 | 253.358 | 254.933 | 256.540 | |
| 0.29614 | 248.794 | 250.251 | 251.738 | 253.253 | 254.798 | 256.375 | 257.977 | 259.612 | |
| 0.40516 | 251.830 | 253.318 | 254.838 | 256.384 | 257.959 | 259.562 | 261.198 | 262.863 | |
| 0.49698 | 254.406 | 255.913 | 257.453 | 259.021 | 260.620 | 262.252 | 263.916 | 265.609 | |
| 0.59993 | 257.267 | 258.800 | 260.366 | 261.964 | 263.593 | 265.256 | 266.948 | 268.674 | |
| 0.69763 | 259.938 | 261.504 | 263.099 | 264.726 | 266.381 | 268.072 | 269.797 | 271.556 | |
| 0.80471 | 262.890 | 264.479 | 266.104 | 267.760 | 269.448 | 271.172 | 272.926 | 274.718 | |
| 0.89712 | 265.336 | 266.956 | 268.609 | 270.299 | 272.012 | 273.764 | 275.547 | 277.368 | |
| 1 | 268.044 | 269.683 | 271.360 | 273.068 | 274.811 | 276.595 | 278.397 | 280.252 | |

^a Standard uncertainties u : $u(T) = 0.05$ °C; $u(x_i) = 0.00006$; $u(V_M) = 0.028$ cm³·mol⁻¹.

Table 22. Dependences of the liquid molar volume V_M on trans-perfluorodecalin (1)–cis-perfluorodecalin (2) system composition x_i at temperature T ^a.

| x_1 | $T/^\circ\text{C}$ | | | | | | | | |
|---------|---------------------------------------|---------|---------|---------|---------|---------|---------|---------|--|
| | 25 | 30 | 35 | 40 | 45 | 50 | 55 | 60 | |
| | $V_M/\text{cm}^3\cdot\text{mol}^{-1}$ | | | | | | | | |
| 0 | 237.435 | 238.826 | 240.240 | 241.676 | 243.099 | 244.606 | 246.124 | 247.663 | |
| 0.10198 | 237.709 | 239.094 | 240.506 | 241.946 | 243.406 | 244.896 | 246.407 | 247.950 | |
| 0.19411 | 237.967 | 239.348 | 240.759 | 242.197 | 243.662 | 245.152 | 246.666 | 248.210 | |
| 0.30439 | 238.268 | 239.654 | 241.067 | 242.506 | 243.974 | 245.469 | 246.989 | 248.538 | |
| 0.41417 | 238.590 | 239.983 | 241.401 | 242.843 | 244.311 | 245.803 | 247.324 | 248.872 | |
| 0.49848 | 238.857 | 240.244 | 241.661 | 243.103 | 244.573 | 246.069 | 247.590 | 249.140 | |
| 0.60085 | 239.147 | 240.536 | 241.955 | 243.399 | 244.870 | 246.368 | 247.892 | 249.441 | |
| 0.70172 | 239.438 | 240.830 | 242.250 | 243.691 | 245.163 | 246.660 | 248.185 | 249.734 | |
| 0.80539 | 239.743 | 241.130 | 242.549 | 243.994 | 245.465 | 246.962 | 248.489 | 250.045 | |
| 0.90273 | 240.007 | 241.396 | 242.817 | 244.263 | 245.736 | 247.240 | 248.770 | 250.325 | |
| 1 | 240.236 | 241.657 | 243.089 | 244.539 | 246.015 | 247.516 | 249.043 | 250.601 | |

^a Standard uncertainties u : $u(T) = 0.05$ °C; $u(x_i) = 0.00006$; $u(V_M) = 0.014$ cm³·mol⁻¹.

Table 23. Dependences of the excess molar volume V^E on perfluoro(butylcyclohexane) (1)–cis-perfluorodecalin (2) system composition x_i at temperature T ^a.

| x_1 | $T/^\circ\text{C}$ | | | | | | | | | |
|---------|---------------------------------------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| | 15 | 20 | 25 | 30 | 35 | 40 | 45 | 50 | 55 | 60 |
| | $V^E/\text{cm}^3\cdot\text{mol}^{-1}$ | | | | | | | | | |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0.10343 | 0.216 | 0.194 | 0.183 | 0.179 | 0.175 | 0.172 | 0.164 | 0.177 | 0.167 | 0.165 |
| 0.17164 | 0.385 | 0.351 | 0.332 | 0.324 | 0.316 | 0.309 | 0.301 | 0.313 | 0.304 | 0.297 |
| 0.28538 | 0.491 | 0.460 | 0.440 | 0.428 | 0.418 | 0.409 | 0.398 | 0.404 | 0.395 | 0.383 |

| | | | | | | | | | | |
|---------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| 0.31744 | 0.478 | 0.454 | 0.438 | 0.433 | 0.424 | 0.423 | 0.408 | 0.404 | 0.392 | 0.379 |
| 0.35826 | 0.516 | 0.479 | 0.459 | 0.448 | 0.438 | 0.427 | 0.417 | 0.418 | 0.405 | 0.391 |
| 0.37933 | 0.513 | 0.485 | 0.470 | 0.462 | 0.453 | 0.440 | 0.428 | 0.426 | 0.411 | 0.394 |
| 0.39919 | 0.551 | 0.517 | 0.497 | 0.487 | 0.475 | 0.468 | 0.454 | 0.455 | 0.443 | 0.427 |
| 0.44022 | 0.546 | 0.512 | 0.490 | 0.479 | 0.467 | 0.458 | 0.443 | 0.444 | 0.433 | 0.418 |
| 0.50224 | 0.510 | 0.477 | 0.459 | 0.448 | 0.437 | 0.428 | 0.416 | 0.417 | 0.404 | 0.392 |
| 0.60547 | 0.524 | 0.484 | 0.462 | 0.453 | 0.442 | 0.434 | 0.423 | 0.418 | 0.413 | 0.397 |
| 0.69350 | 0.479 | 0.457 | 0.447 | 0.445 | 0.440 | 0.433 | 0.426 | 0.422 | 0.415 | 0.404 |
| 0.80202 | 0.392 | 0.362 | 0.345 | 0.342 | 0.336 | 0.336 | 0.329 | 0.329 | 0.331 | 0.322 |
| 0.88860 | 0.295 | 0.269 | 0.256 | 0.259 | 0.256 | 0.258 | 0.256 | 0.254 | 0.260 | 0.257 |
| 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

^a Standard uncertainties u : $u(T) = 0.05$ °C; $u(x_i) = 0.00005$; $u(V^E) = 0.034$ cm³·mol⁻¹.

Table 24. Dependences of the excess molar volume V^E on perfluoro(butylcyclohexane) (1)–trans-perfluorodecalin (2) system composition x_i at temperature T ^a.

| x_1 | $T/^\circ\text{C}$ | | | | | | | | |
|---------|---------------------------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| | 25 | 30 | 35 | 40 | 45 | 50 | 55 | 60 | |
| | $V^E/\text{cm}^3\cdot\text{mol}^{-1}$ | | | | | | | | |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0.10688 | 0.150 | 0.123 | 0.109 | 0.102 | 0.096 | 0.093 | 0.090 | 0.087 | 0.087 |
| 0.19419 | 0.272 | 0.239 | 0.220 | 0.211 | 0.202 | 0.195 | 0.190 | 0.181 | 0.181 |
| 0.29614 | 0.323 | 0.294 | 0.277 | 0.265 | 0.255 | 0.248 | 0.241 | 0.230 | 0.230 |
| 0.40516 | 0.327 | 0.306 | 0.295 | 0.286 | 0.277 | 0.264 | 0.262 | 0.249 | 0.249 |
| 0.49698 | 0.350 | 0.328 | 0.314 | 0.304 | 0.294 | 0.284 | 0.285 | 0.272 | 0.272 |
| 0.59993 | 0.348 | 0.329 | 0.316 | 0.310 | 0.302 | 0.295 | 0.295 | 0.284 | 0.284 |
| 0.69763 | 0.302 | 0.295 | 0.287 | 0.284 | 0.277 | 0.270 | 0.276 | 0.270 | 0.270 |
| 0.80471 | 0.277 | 0.269 | 0.265 | 0.263 | 0.261 | 0.256 | 0.262 | 0.257 | 0.257 |
| 0.89712 | 0.153 | 0.156 | 0.158 | 0.166 | 0.164 | 0.161 | 0.170 | 0.166 | 0.166 |
| 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

^a Standard uncertainties u : $u(T) = 0.05$ °C; $u(x_i) = 0.00006$; $u(V^E) = 0.038$ cm³·mol⁻¹.

Table 25. Dependences of the excess molar volume V^E on trans-perfluorodecalin (1)–cis-perfluorodecalin (2) system composition x_i at temperature T ^a.

| x_1 | $T/^\circ\text{C}$ | | | | | | | | |
|---------|---------------------------------------|--------|--------|--------|--------|--------|--------|--------|--------|
| | 25 | 30 | 35 | 40 | 45 | 50 | 55 | 60 | |
| | $V^E/\text{cm}^3\cdot\text{mol}^{-1}$ | | | | | | | | |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0.10198 | -0.012 | -0.021 | -0.025 | -0.022 | 0.010 | -0.007 | -0.015 | -0.013 | -0.013 |
| 0.19411 | -0.012 | -0.028 | -0.034 | -0.035 | -0.003 | -0.019 | -0.025 | -0.023 | -0.023 |
| 0.30439 | -0.020 | -0.034 | -0.040 | -0.041 | -0.013 | -0.023 | -0.024 | -0.019 | -0.019 |
| 0.41417 | -0.005 | -0.016 | -0.019 | -0.019 | 0.004 | -0.008 | -0.009 | -0.008 | -0.008 |
| 0.49848 | 0.026 | 0.007 | 0.001 | 0 | 0.020 | 0.012 | 0.011 | 0.012 | 0.012 |
| 0.60085 | 0.029 | 0.009 | 0.003 | 0.003 | 0.019 | 0.014 | 0.014 | 0.013 | 0.013 |
| 0.70172 | 0.037 | 0.017 | 0.011 | 0.006 | 0.018 | 0.012 | 0.013 | 0.009 | 0.009 |
| 0.80539 | 0.052 | 0.024 | 0.014 | 0.012 | 0.017 | 0.012 | 0.014 | 0.016 | 0.016 |
| 0.90273 | 0.043 | 0.014 | 0.005 | 0.002 | 0.005 | 0.007 | 0.011 | 0.010 | 0.010 |
| 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

^a Standard uncertainties u : $u(T) = 0.05$ °C; $u(x_i) = 0.00006$; $u(V^E) = 0.025$ cm³·mol⁻¹.

The excess molar volume data (Tables 23–25) were correlated with the Redlich-Kister [138] Equation (9a). The Redlich-Kister parameters are presented in Tables 26–28. The

standard deviation σ between experimental (Tables 23–25) and calculated by Equation (9a) (Tables 26–28, accordingly) data were calculated according to Equation (9b) [139].

$$V^E = x_1 x_2 \sum_{i=0}^i a_i (x_1 - x_2)^i \quad (9a)$$

$$\sigma(V^E) = \sqrt{\frac{\sum (V_{exp}^E - V_{calc}^E)^2}{d - \bar{n}}} \quad (9b)$$

where a_i represents the Redlich-Kister parameters; d is the number of compositions studied; \bar{n} represents the number of terms used in the regression.

Table 26. Redlich-Kister regression results (according to the Equation (9a,b)) for the excess molar volumes V^E at temperature T of perfluoro(butylcyclohexane) (1)–cis-perfluorodecalin (2) system calculated from Table 23 data.

| $T/^\circ\text{C}$ | a_3 | a_2 | a_1 | a_0 | $\sigma(V^E)/\text{cm}^3\cdot\text{mol}^{-1}$ |
|--------------------|----------|----------|-----------|----------|---|
| 15 | 1.104964 | 0.978578 | −0.344386 | 2.129725 | 0.021 |
| 20 | 1.062583 | 0.771174 | −0.326034 | 2.008629 | 0.019 |
| 25 | 1.006494 | 0.675298 | −0.295903 | 1.938418 | 0.018 |
| 30 | 1.054220 | 0.720329 | −0.277812 | 1.898207 | 0.018 |
| 35 | 1.042090 | 0.725251 | −0.260297 | 1.856007 | 0.018 |
| 40 | 1.097235 | 0.774554 | −0.255016 | 1.817599 | 0.018 |
| 45 | 1.136660 | 0.774213 | −0.243640 | 1.767653 | 0.018 |
| 50 | 0.985911 | 0.886383 | −0.249339 | 1.755389 | 0.018 |
| 55 | 1.124080 | 0.934376 | −0.232019 | 1.709023 | 0.019 |
| 60 | 1.098612 | 0.985980 | −0.221599 | 1.644507 | 0.018 |

Table 27. Redlich-Kister regression results (according to Equation (9a,b)) for the excess molar volumes V^E at temperature T of perfluoro(butylcyclohexane) (1)–trans-perfluorodecalin (2) system calculated from Table 24 data.

| $T/^\circ\text{C}$ | a_4 | a_3 | a_2 | a_1 | a_0 | $\sigma(V^E)/\text{cm}^3\cdot\text{mol}^{-1}$ |
|--------------------|-----------|----------|----------|-----------|----------|---|
| 25 | −1.954153 | 0.190090 | 1.674633 | −0.058943 | 1.343112 | 0.018 |
| 30 | −1.845871 | 0.425479 | 1.529335 | −0.003537 | 1.264095 | 0.014 |
| 35 | −1.727888 | 0.544906 | 1.430764 | 0.021673 | 1.215389 | 0.013 |
| 40 | −1.492634 | 0.699904 | 1.345204 | 0.020418 | 1.183338 | 0.012 |
| 45 | −1.502029 | 0.689572 | 1.344187 | 0.056314 | 1.146885 | 0.012 |
| 50 | −1.512829 | 0.657437 | 1.354771 | 0.072389 | 1.106092 | 0.012 |
| 55 | −1.334099 | 0.710743 | 1.304439 | 0.124689 | 1.104640 | 0.012 |
| 60 | −1.295411 | 0.631341 | 1.298648 | 0.165574 | 1.060024 | 0.010 |

Table 28. Redlich-Kister regression results (according to Equation (9a,b)) for the excess molar volumes V^E at temperature T of trans-perfluorodecalin (1)–cis-perfluorodecalin (2) system calculated from Table 25 data.

| $T/^\circ\text{C}$ | a_1 | a_0 | $\sigma(V^E)/\text{cm}^3\cdot\text{mol}^{-1}$ |
|--------------------|----------|-----------|---|
| 25 | 0.363697 | 0.099868 | 0.011 |
| 30 | 0.259612 | −0.019726 | 0.006 |
| 35 | 0.232529 | −0.060487 | 0.008 |
| 40 | 0.205715 | −0.066386 | 0.009 |
| 45 | 0.093063 | 0.034057 | 0.010 |
| 50 | 0.135899 | −0.002282 | 0.008 |
| 55 | 0.194350 | −0.010696 | 0.007 |
| 60 | 0.175727 | −0.005742 | 0.006 |

The dependences for the excess molar volume of the BCH–cis-PFD, BCH–trans-PFD and trans-PFD–cis-PFD systems on composition and temperature were correlated using Equation (10a,b); the parameters were calculated from Tables 26–28 data and are listed in Tables 29–31. The standard deviation σ (Equation (9b)) between experimental (Tables 23–25) and calculated by Equation (10a,b) (Tables 29–31) data for each temperature are given in Appendix A (Tables A7–A9, respectively).

$$V^E = x_1 x_2 \sum_{i=0}^i a_i (x_1 - x_2)^i \quad (10a)$$

$$a_i = \sum_{j=0}^j b_j T^j \quad (10b)$$

where a_i is the temperature-depended Redlich-Kister parameters; x is the composition of the binary system; b_j represents the parameters of Equation (10b); T is the temperature, °C.

Table 29. Redlich-Kister regression results (according to Equation (10a,b)) for the excess molar volumes V^E of perfluoro(butylcyclohexane) (1)–cis-perfluorodecalin (2) system calculated from Table 26 data ^a.

| a_i | b_j | | |
|-------|-----------|-----------|-----------|
| | b_2 | b_1 | b_0 |
| a_3 | 0.000072 | −0.004674 | 1.131143 |
| a_2 | 0.000478 | −0.032840 | 1.283535 |
| a_1 | −0.000052 | 0.006427 | −0.428262 |
| a_0 | 0.000105 | −0.017362 | 2.333832 |

^a $\sigma(V^E) = 0.017 \text{ cm}^3 \cdot \text{mol}^{-1}$.

Table 30. Redlich-Kister regression results (according to Equation (10a,b)) for the excess molar volumes V^E of perfluoro(butylcyclohexane) (1)–trans-perfluorodecalin (2) system calculated from Table 27 data ^a.

| a_i | b_j | | |
|-------|-----------|-----------|-----------|
| | b_2 | b_1 | b_0 |
| a_4 | −0.000293 | 0.043508 | −2.864105 |
| a_3 | −0.000873 | 0.085766 | −1.384216 |
| a_2 | 0.000439 | −0.046791 | 2.548607 |
| a_1 | 0.000048 | 0.001634 | −0.112666 |
| a_0 | 0.000137 | −0.019123 | 1.725379 |

^a $\sigma(V^E) = 0.010 \text{ cm}^3 \cdot \text{mol}^{-1}$.

Table 31. Redlich-Kister regression results (according to Equation (10a,b)) for the excess molar volumes V^E of trans-perfluorodecalin (1)–cis-perfluorodecalin (2) system calculated from Table 28 data ^a.

| a_i | b_j | | |
|-------|----------|-----------|----------|
| | b_2 | b_1 | b_0 |
| a_1 | 0.000388 | −0.037870 | 1.064833 |
| a_0 | 0.000233 | −0.020799 | 0.428681 |

^a $\sigma(V^E) = 0.010 \text{ cm}^3 \cdot \text{mol}^{-1}$.

Comparisons of the experimental (Tables 23–25) and calculated by Equation (9a) (Tables 26–28) or Equation (10) (Tables 29–31) data for the BCH–cis-PFD, BCH–trans-PFD, and trans-PFD–cis-PFD systems are presented in Figures 15–17, respectively.

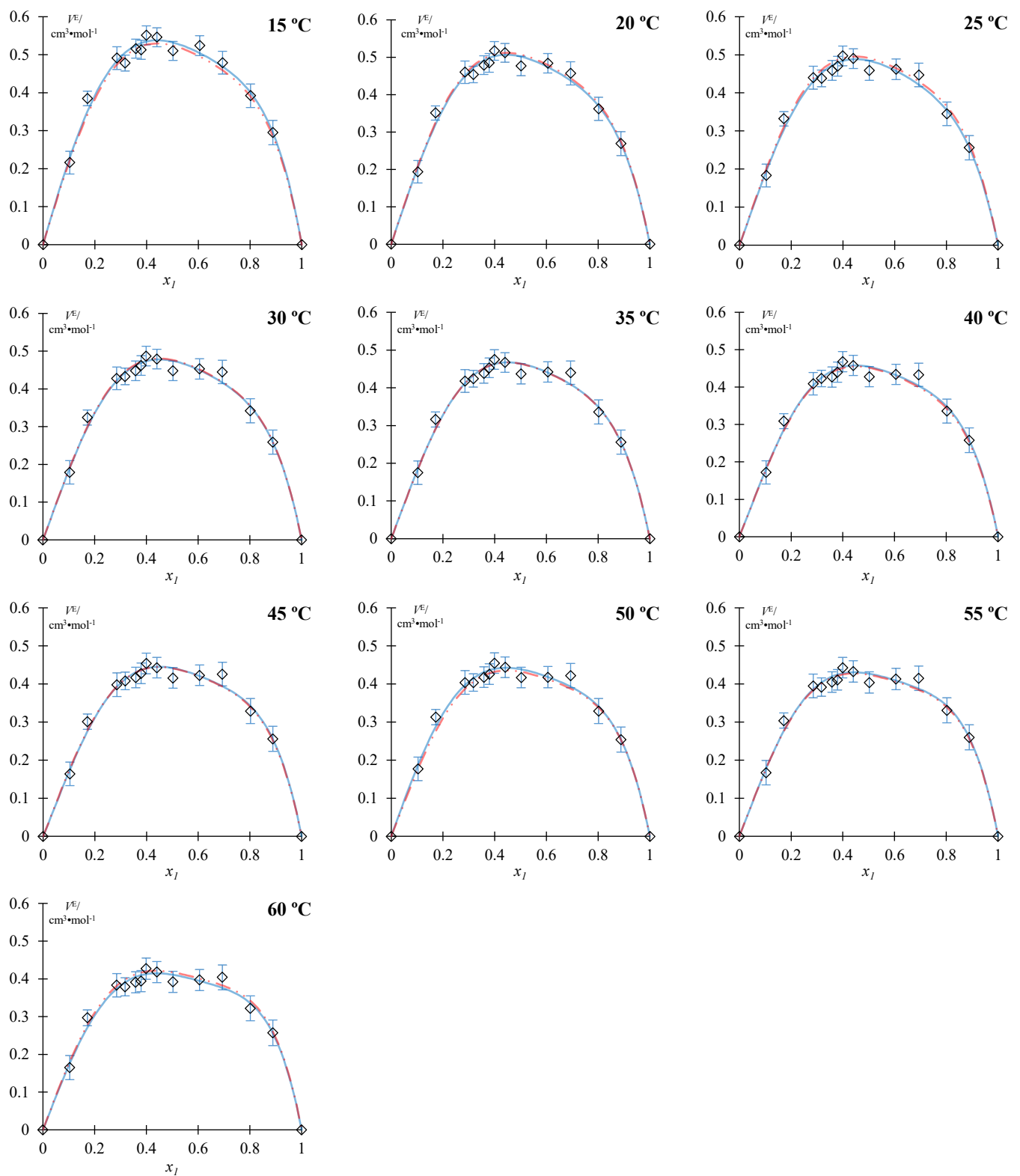


Figure 15. Dependences of the excess molar volume V^E versus concentration x_i in the perfluoro(butylcyclohexane) (1)–cis-perfluorodecalin (2) system at temperature T . Points: experimental data according to Table 23; lines: calculated data according to the Redlich-Kister equation; red: Equation (9a)—Table 26; blue: Equation (10a,b)—Table 29.

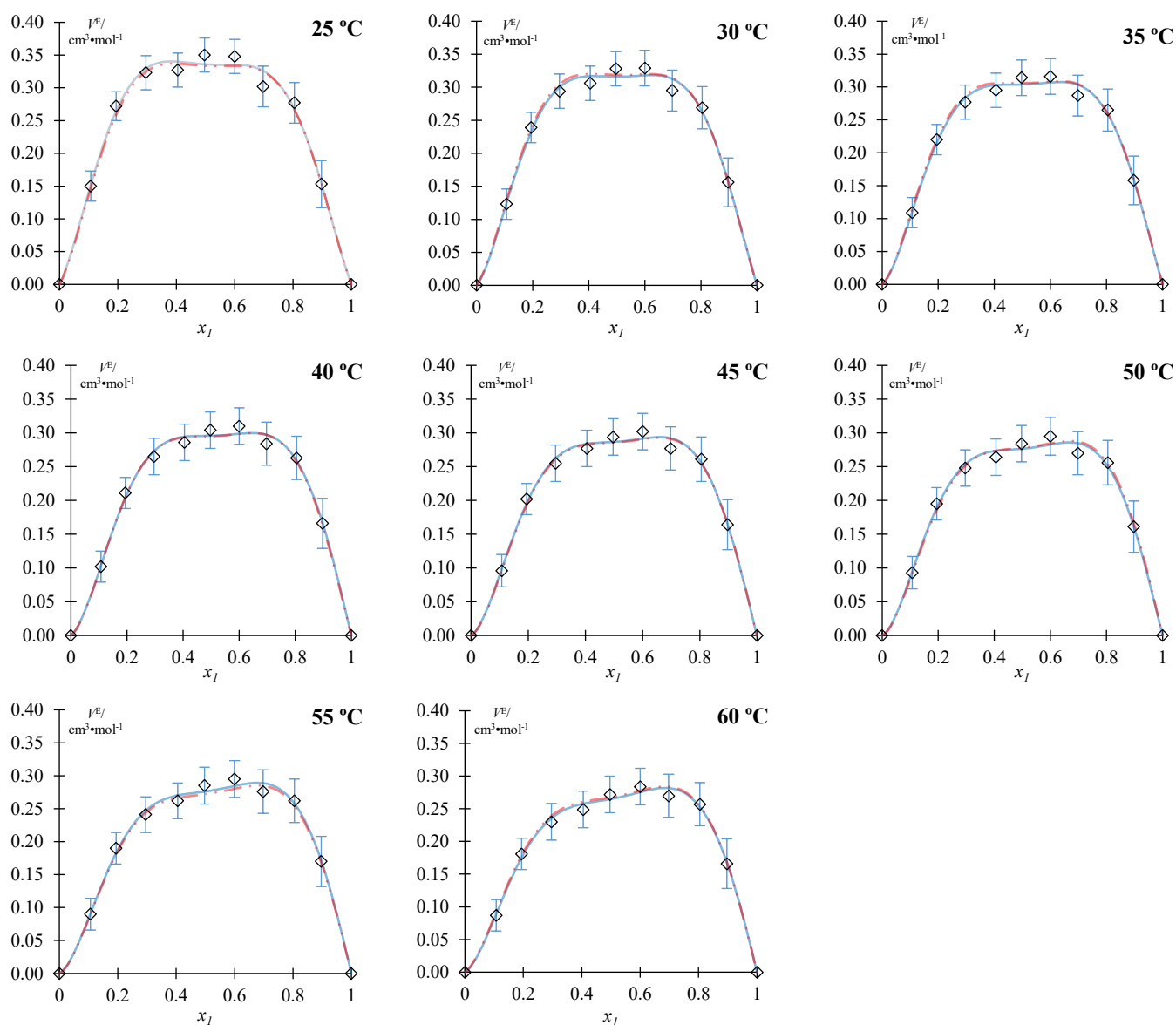
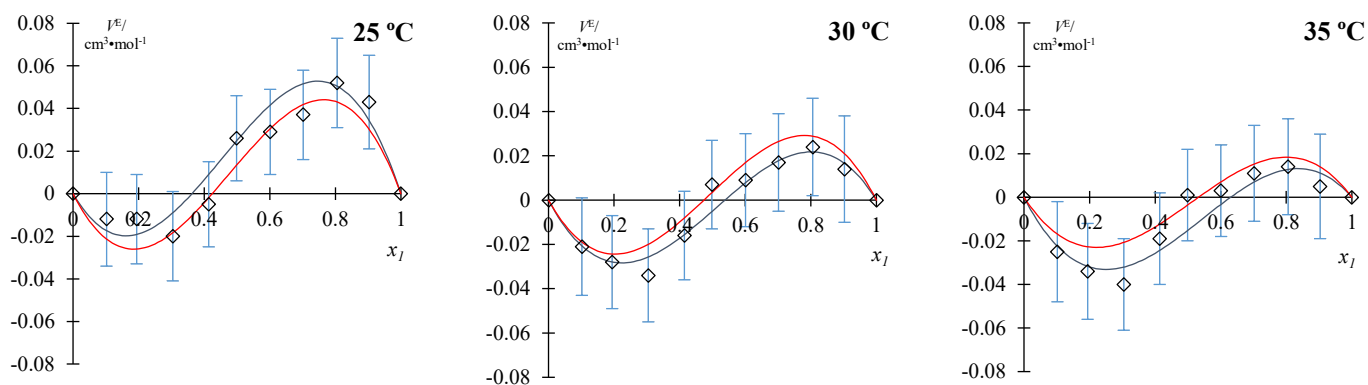


Figure 16. Dependences of the excess molar volume V^E versus concentration x_1 in the perfluoro(butylcyclohexane) (1)–trans-perfluorodecalin (2) system at temperature T . Points: experimental data according to Table 24; lines: calculated data according to the Redlich-Kister equation; red: Equation (9a)–Table 27; blue: Equation (10a,b)–Table 30.



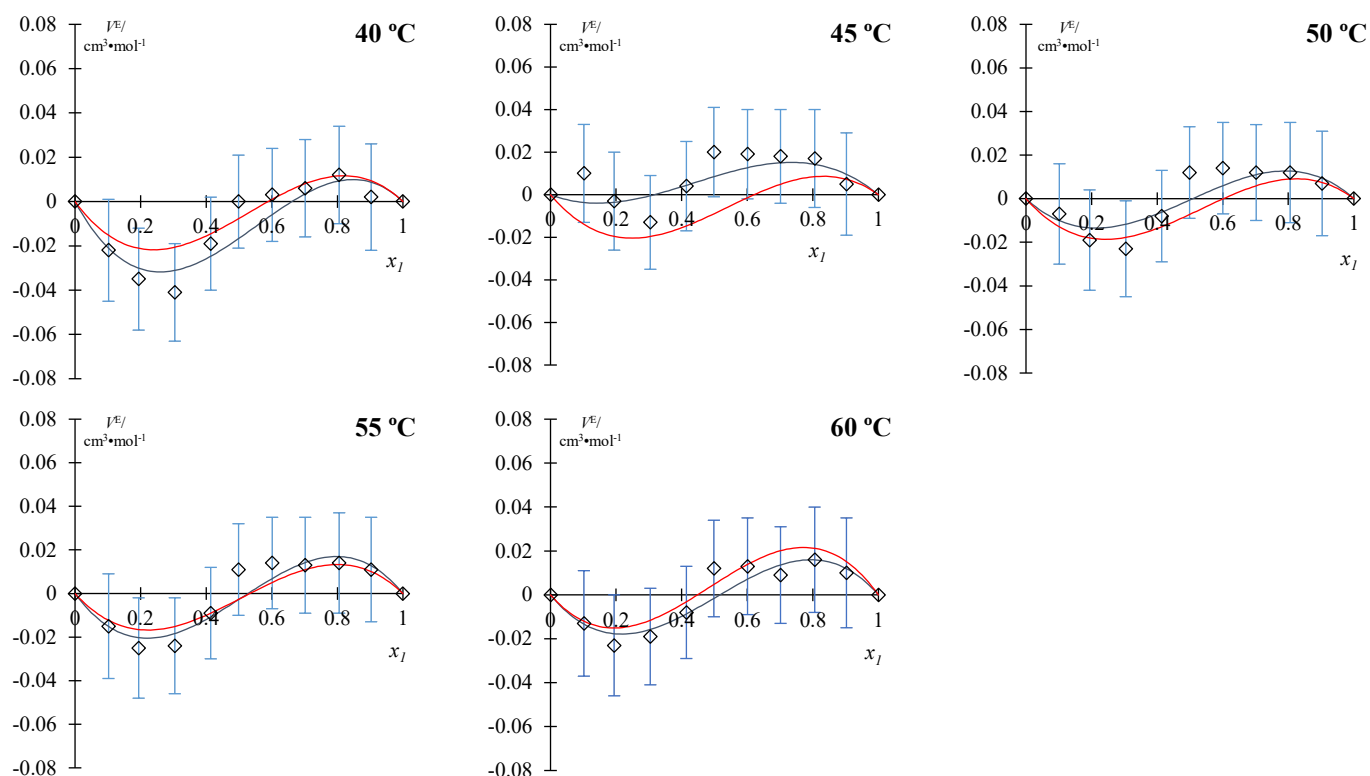


Figure 17. Dependences of the excess molar volume V^E versus concentration x_i in the trans-perfluorodecalin (1)–cis-perfluorodecalin (2) system at temperature T . Points: experimental data according to Table 25; lines: calculated data according to the Redlich-Kister equation; red: Equation (9a)–Table 28; blue: Equation (10a,b)–Table 31.

3.7.3. Ternary System

The dependence of the density ρ on BCH–trans-PFD–cis-PFD system composition at different temperatures is presented in Table 32. The liquid molar volume, V_M , of the BCH–trans-PFD–cis-PFD system was calculated according to Equation (7) and is presented in Table 33. Excess molar volume V^E of the BCH–trans-PFD–cis-PFD system was calculated according to Equation (8) and is presented in Table 34 and Figure 18. The V_M and V^E data (Tables 33 and 34) provides the maximum standard uncertainties, u , of the values; standard uncertainties, u , for each experimental point are given in Appendix A (Tables A10 and A11, respectively).

Table 32. Dependences of density ρ on perfluoro(butylcyclohexane) (1)–trans-perfluorodecalin (2)–cis-perfluorodecalin (3) system composition x_i at temperature T and pressure $P = 99.1$ kPa ^a.

| x_1 | x_2 | x_3 | $T/^\circ\text{C}$ | | | | | | | |
|---------|---------|---------|------------------------------------|---------|---------|---------|---------|---------|---------|---------|
| | | | 25 | 30 | 35 | 40 | 45 | 50 | 55 | 60 |
| | | | $\rho/\text{g}\cdot\text{cm}^{-3}$ | | | | | | | |
| 0.57402 | 0.21988 | 0.20610 | 1.89013 | 1.87891 | 1.86761 | 1.85623 | 1.84481 | 1.83331 | 1.82175 | 1.81008 |
| 0.17479 | 0.19519 | 0.63002 | 1.92382 | 1.91265 | 1.90139 | 1.89007 | 1.87867 | 1.86720 | 1.85569 | 1.84408 |
| 0.17937 | 0.63244 | 0.18819 | 1.91397 | 1.90288 | 1.89168 | 1.88044 | 1.86911 | 1.85769 | 1.84621 | 1.83466 |
| 0.18870 | 0.39863 | 0.41267 | 1.91787 | 1.90673 | 1.89552 | 1.88424 | 1.87287 | 1.86144 | 1.84997 | 1.83842 |
| 0.36974 | 0.40875 | 0.22151 | 1.90212 | 1.89101 | 1.87981 | 1.86853 | 1.85715 | 1.84571 | 1.83419 | 1.82261 |
| 0.37885 | 0.22255 | 0.39860 | 1.90497 | 1.89385 | 1.88261 | 1.87129 | 1.85991 | 1.84846 | 1.83691 | 1.82532 |

^a Standard uncertainties u : $u(T) = 0.05$ °C; $u(x_i) = 0.00005$; $u(\rho) = 0.0001$ g·cm⁻³; $u(P) = 0.3$ kPa.

Table 33. Dependences of the liquid molar volume V_M on perfluoro(butylcyclohexane) (1)–trans-perfluorodecalin (2)–cis-perfluorodecalin (3) system composition x_i at temperature T^a .

| x_1 | x_2 | x_3 | $T/^\circ\text{C}$ | | | | | | | |
|---------|---------|---------|---------------------------------------|---------|---------|---------|---------|---------|---------|---------|
| | | | 25 | 30 | 35 | 40 | 45 | 50 | 55 | 60 |
| | | | $V_M/\text{cm}^3\cdot\text{mol}^{-1}$ | | | | | | | |
| 0.57402 | 0.21988 | 0.20610 | 256.007 | 257.536 | 259.094 | 260.683 | 262.296 | 263.942 | 265.617 | 267.329 |
| 0.17479 | 0.19519 | 0.63002 | 243.640 | 245.063 | 246.515 | 247.991 | 249.496 | 251.028 | 252.585 | 254.176 |
| 0.17937 | 0.63244 | 0.18819 | 244.988 | 246.416 | 247.875 | 249.356 | 250.868 | 252.410 | 253.979 | 255.578 |
| 0.18870 | 0.39863 | 0.41267 | 244.669 | 246.099 | 247.554 | 249.036 | 250.548 | 252.087 | 253.650 | 255.243 |
| 0.36974 | 0.40875 | 0.22151 | 250.314 | 251.784 | 253.284 | 254.813 | 256.375 | 257.964 | 259.584 | 261.233 |
| 0.37885 | 0.22255 | 0.39860 | 250.121 | 251.589 | 253.091 | 254.622 | 256.180 | 257.767 | 259.388 | 261.035 |

^a Standard uncertainties u : $u(T) = 0.05$ °C; $u(x_i) = 0.00005$; $u(V_M) = 0.024$ cm³·mol^{−1}.

Table 34. Dependences of the excess molar volume V^E on perfluoro(butylcyclohexane) (1)–trans-perfluorodecalin (2)–cis-perfluorodecalin (3) system composition x_i at temperature T^a .

| x_1 | x_2 | x_3 | $T/^\circ\text{C}$ | | | | | | | |
|---------|---------|---------|---------------------------------------|-------|-------|-------|-------|-------|-------|-------|
| | | | 25 | 30 | 35 | 40 | 45 | 50 | 55 | 60 |
| | | | $V^E/\text{cm}^3\cdot\text{mol}^{-1}$ | | | | | | | |
| 0.57402 | 0.21988 | 0.20610 | 0.386 | 0.375 | 0.364 | 0.358 | 0.353 | 0.334 | 0.326 | 0.313 |
| 0.17479 | 0.19519 | 0.63002 | 0.308 | 0.291 | 0.279 | 0.269 | 0.285 | 0.263 | 0.250 | 0.243 |
| 0.17937 | 0.63244 | 0.18819 | 0.289 | 0.262 | 0.248 | 0.236 | 0.234 | 0.223 | 0.217 | 0.209 |
| 0.18870 | 0.39863 | 0.41267 | 0.344 | 0.324 | 0.308 | 0.297 | 0.305 | 0.287 | 0.275 | 0.262 |
| 0.36974 | 0.40875 | 0.22151 | 0.417 | 0.392 | 0.373 | 0.360 | 0.359 | 0.341 | 0.334 | 0.320 |
| 0.37885 | 0.22255 | 0.39860 | 0.466 | 0.443 | 0.427 | 0.416 | 0.418 | 0.394 | 0.388 | 0.372 |

^a Standard uncertainties u : $u(T) = 0.05$ °C; $u(x_i) = 0.00005$; $u(V^E) = 0.189$ cm³·mol^{−1}.

The excess molar volume data (Table 34) of the BCH–trans-PFD–cis-PFD system were correlated with the Kohler [140,141] Equation (11); the data calculated by Equation (11) for the BCH–trans-PFD–cis-PFD system are presented in Table 35. The standard deviation σ (Equation (9b)) between experimental (Table 34) and calculated by Equation (11) (Table 35) data for each temperature are given in Appendix A (Table A12).

$$V^E = \sum_{i \neq j; i, j=1}^{i, j} (x_i + x_j)^2 V_{ij}^E \quad (11)$$

where $V_{ij}^E = x_i' x_j' \sum_{l=0}^l a_l (x_i' - x_j')^l$ indicates that the excess molar volume of the pseudo-binary system with composition $x_i' = x_i / (x_i + x_j)$ and $x_j' = x_j / (x_i + x_j)$; $a_l = \sum_{j=0}^j b_j T^j$ indicates that the temperature depended Redlich-Kister parameters; x_i represents the composition of the ternary system; b_j is calculated from binary system data parameters (listed in Tables 29–31); T represents the temperature, °C.

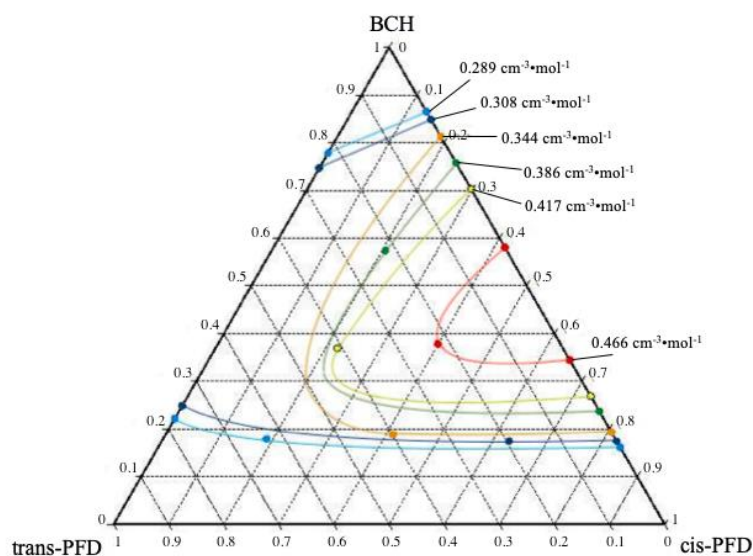


Figure 18. Dependence of the isoline of excess molar volume V^E on perfluoro(butylcyclohexane) (BCH)–trans-perfluorodecalin (trans-PFD)–cis-perfluorodecalin (cis-PFD) system composition at 25 °C according to the Tables 26–28 and 34 data.

Table 35. Calculated by Kohler Equation (11) the excess molar volume V_{calc}^E data for the per-fluoro(butylcyclohexane) (1)–trans-perfluorodecalin (2)–cis-perfluorodecalin (3) system at temperature T and composition x .^a

| x_1 | x_2 | x_3 | $T/^\circ\text{C}$ | | | | | | | |
|---------|---------|---------|--|-------|-------|-------|-------|-------|-------|-------|
| | | | 25 | 30 | 35 | 40 | 45 | 50 | 55 | 60 |
| | | | $V_{calc}^E/\text{cm}^3\cdot\text{mol}^{-1}$ | | | | | | | |
| 0.57402 | 0.21988 | 0.20610 | 0.452 | 0.437 | 0.425 | 0.415 | 0.409 | 0.405 | 0.403 | 0.405 |
| 0.17479 | 0.19519 | 0.63002 | 0.270 | 0.260 | 0.251 | 0.245 | 0.241 | 0.238 | 0.238 | 0.239 |
| 0.17937 | 0.63244 | 0.18819 | 0.283 | 0.257 | 0.235 | 0.219 | 0.208 | 0.201 | 0.199 | 0.203 |
| 0.18870 | 0.39863 | 0.41267 | 0.288 | 0.270 | 0.255 | 0.243 | 0.235 | 0.231 | 0.229 | 0.231 |
| 0.36974 | 0.40875 | 0.22151 | 0.377 | 0.358 | 0.341 | 0.328 | 0.318 | 0.311 | 0.308 | 0.307 |
| 0.37885 | 0.22255 | 0.39860 | 0.414 | 0.399 | 0.386 | 0.375 | 0.366 | 0.360 | 0.355 | 0.352 |

^a $\sigma(V^E) = 0.049 \text{ cm}^3\cdot\text{mol}^{-1}$.

4. Discussion

4.1. Spectrum Data

To verify the structures and molecular weights of the studied components, GC-MS and NMR data were obtained.

Based on the analysis of the trans-PFD and cis-PFD gas chromatography–mass spectrometry data (Figure 2), it follows that both samples weighed $462 \text{ g}\cdot\text{mol}^{-1}$ and the fragmentation patterns included standard fragmentation ($93\text{—}[\text{C}_3\text{F}_3]$, $131\text{—}[\text{C}_3\text{F}_5]$, $443\text{—}[\text{C}_{10}\text{F}_{17}]$ and $462\text{—}\text{C}_{10}\text{F}_{18}$ for example), although the intensity of the patterns differed slightly from those in the literature [142]. The ^{19}F NMR spectra of the trans-PFD and cis-PFD (Figure 3b) corresponded to that reported previously [63]. Despite the fact that the ^{19}F spectrum of the cis-PFD was more complex than that for trans-PFD (Figure 3b), their ^{13}C spectra were similar (Figure 3a). The fingerprint region of trans-PFD and cis-PFD FTIR spectra are presented in Figure 4. The FTIR spectra were relatively similar if the wave numbers were overlooked (Figure 4c). The characteristic peaks of trans-PFD and cis-PFD (Figure 4) corresponded to those in the literature [115]. Meanwhile, the relative intensity of the characteristic trans-PFD and cis-PFD peaks near 1250 cm^{-1} did not agree with those reported by Bris et al. [115]. However, a more detailed analysis of gas chromatography–mass spectrometry data (Figure 2) via NMR (Figure 3) and FTIR (Figure 4) was not

provided as their interpretation is difficult and is a separate scientific task. As the data seem to be useful, the «.mzxml», «.dx» and «.ispd» original files are provided.

4.2. Differential Scanning Calorimetry Data

Based on the analysis of the DSC data (Figure 5 and Table 2), in the case of the cis-PFD at cooling and heating, a considerable difference was observed between onset points of crystallization and melting ($T_c = -17.20$ °C and $T_m = -6.99$ °C); moreover, the crystallization average point was outside the onset and endset of the heat effect ($T_c^{endset} < T_c^{onset} < T_c^{average}$). The same situation occurred in the case of trans-PFD ($T_c = 3.48$ °C and $T_m = 21.22$ °C; $T_c^{endset} < T_c^{onset} < T_c^{average}$). The observed difference may be caused by low thermal conductivity, difficulties forming a solid phase nucleus (crystallization centers), and the resulting supercooling. However, the obtained experimental data on solid–liquid phase transition ($T_m^{cis-PFD} = -6.99$ °C and $T_m^{trans-PFD} = 21.22$ °C) and its heat effect ($\Delta H_m^{cis-PFD} = 21.35$ J·g⁻¹ and $\Delta H_m^{trans-PFD} = 38.41$ J·g⁻¹) agree with that presented in the literature [143] ($T_m^{cis-PFD} = -6.55$ °C and $T_m^{trans-PFD} = 21.46$ °C; $\Delta H_m^{cis-PFD} = 22.30$ J·g⁻¹ and $\Delta H_m^{trans-PFD} = 38.87$ J·g⁻¹). The melting temperature data were also presented by Smith [123] ($T_m^{cis-PFD} = -7.0$ °C and $T_m^{trans-PFD} = 17.5$ °C), however, the samples exhibited low purity (cis-PFD [123] > 95% mass., trans-PFD [123] > 90% mass.).

Following cooling and heating of the samples among the crystallization and melting characteristic peaks, the DSC data showed additional heat effects:

- In the case of cis-PFD heating, two effects were absent during cooling. The first (−39.11 °C) correlates to the solid–solid phase transition (c_{II}/c_I) temperature [143] (−40.65 °C); their heat effects differed ($\Delta H_{c_{II}/c_I}^{exp} = 0.60$ J·g⁻¹ and $\Delta H_{c_{II}/c_I}^{lit} = 9.18$ J·g⁻¹). The second belongs to the −95.69 °C to −87.60 °C temperature range and is not found in the literature; it likely corresponds to the glass transition effect. The conclusion agrees with the $T_g/T_m = 2/3$ empirical rule [144], where the temperature is in Kelvin scale.
- In the case of trans-PFD cooling, there is a relaxation effect at −0.90 °C subsequent to the crystallization caused by supercooling. In the case of trans-PFD heating, there is a heat effect in the temperature range from −96.57 °C to −85.87 °C, which is absent during cooling. This likely corresponds to the glass transition effect that agrees with the two-thirds empirical rule [144].

4.3. Viscosity

The data obtained in the present work for trans-PFD and cis-PFD are equivalent to those previously reported for BCH and MBCN [130]. The compounds showed Newtonian behavior (Figure 6), with «zero» shear viscosity values of $\eta_{trans-PFD}^{25\text{ °C}} = 49.4 \times 10^{-4}$ Pa·s and $\eta_{cis-PFD}^{25\text{ °C}} = 69.4 \times 10^{-4}$ Pa·s (Table 3). As the temperature increased, the $\eta_{trans-PFD}^T$ and $\eta_{cis-PFD}^T$ values decreased (Figure 7a). The $\eta = f\left(\frac{1}{T}\right)$ function was linear (Figure 7b). The $\eta_{trans-PFD}^T$ and $\eta_{cis-PFD}^T$ data correlated with the Arrhenius Equation (1). The coefficients of the Arrhenius equation are listed in Table 4.

In the case of trans-PFD, crystallization at 9.3 °C was detected during the continuous temperature scanning mode (Figure 8). The rotational rheometry data disagreed with the DSC data (Table 2) as the experiment was carried out under constant shear conditions. At the process's initial stage, the solid phase nucleus (crystallization centers) was destroyed. As a result, the crystallization was detected at lower temperatures.

The dependences of viscosity on the shear rate at 25 °C and temperature of the MBCN, BCH, trans-PFD, and cis-PFD are shown in Figure 9. In the investigated shear rate and temperature ranges, the viscosity order of the components was as follows: $\eta_{cis-PFD} > \eta_{trans-PFD} > \eta_{MBCN} > \eta_{BCH}$.

Deepika [101] provided data on the dependence of the dynamic viscosity at different temperatures ($\eta_{PFD}^{25\text{ °C}} = 56.47$ Pa·s $\times 10^{-4}$, for example) and apparent activation energy ($E_a^{PFD} = 19,920$ J·mol⁻¹) for the viscous flow of the «pure perfluorodecalin» isomeric

composition of which is not given; the data are within the range of values determined in the present work for trans-PFD ($\eta_{trans-PFD}^{25\text{ }^\circ\text{C}} = 49.4 \text{ Pa}\cdot\text{s} \times 10^{-4}$, $E_a^{trans-PFD} = 17,944.3 \text{ J}\cdot\text{mol}^{-1}$) and cis-PFD ($\eta_{cis-PFD}^{25\text{ }^\circ\text{C}} = 69.3 \text{ Pa}\cdot\text{s} \times 10^{-4}$, $E_a^{cis-PFD} = 24,036.6 \text{ J}\cdot\text{mol}^{-1}$) (Tables 3 and 4).

Haszeldine [104] also provides data on PFD viscosity in the 25 to 80 °C range, however, the isomeric composition is not given; the data are similar to the experimental values obtained in the present work for trans-PFD (Table 3): $\Delta\eta_{trans-PFD}^{25\text{ }^\circ\text{C}} = 49.4^{exp} - 51.4^{lit} = -2.0 \text{ Pa}\cdot\text{s} \times 10^{-4}$; $\Delta\eta_{trans-PFD}^{35\text{ }^\circ\text{C}} = 38.2^{exp} - 37.6^{lit} = 0.6 \text{ Pa}\cdot\text{s} \times 10^{-4}$; $\Delta\eta_{trans-PFD}^{45\text{ }^\circ\text{C}} = 31.2^{exp} - 28.6^{lit} = 2.2 \text{ Pa}\cdot\text{s} \times 10^{-4}$. A similar situation was observed when comparing the data from Freire [103] with those in Table 3.

4.4. Saturated Vapor Pressure

The obtained dependences of the saturated vapor pressure for trans-PFD (Table 5) and cis-PFD (Table 6) on temperature showed that T_b difference remained relatively intact $\Delta T_b^P = [0.3; 1.4] \text{ }^\circ\text{C}$; the Antoine Equation (2) and regressed parameters (Table 7) provide a proper correlation of the experimental data (Figure 10a,b). Considering the experimental uncertainty, the measured values for the dependence of saturated vapor pressure on temperature for trans-PFD (Table 5) and cis-PFD (Table 6) were generally in agreement with the literature data [90,123,136,145]. However, there were some inconsistencies for the boiling point row of the components under study: ($T_b^{trans-PFD} < T_b^{cis-PFD} < T_b^{BCH}$) [123,136,145] and ($T_b^{trans-PFD} < T_b^{BCH} < T_b^{cis-PFD}$)^{exp}. Note that in Dias [90] a mixture of trans-PFD and cis-PFD in an unknown ratio was used; in Smith [123] the purity of the investigated samples was relatively low (cis-PFD > 95% mass., trans-PFD > 90% mass.), and in the Gervits [136] and Varushchenko [145] the purity was unspecified.

From Figure 10c, it follows that the $P = f(T)$ dependence of the MBCN significantly differed from other components, and trans-PFD, cis-PFD, and BCH are close-boiling substances. The question of the presence of Bancroft's point for trans-PFD, cis-PFD, and BCH remains unclear, as the temperature uncertainty was within the range of measurable differences. In the case of Bancroft's point being present, the system is characterized by an azeotrope under certain conditions. Moreover, the Bancroft point is a condition for the transition boundary tangential azeotropy to internal tangential azeotropy (and inverse) in the case of binary biazeotropic systems [146].

Since MBCN is a mixture of diastereomers, the ratio changes of which may lead to changes in the properties of the sample, MBCN was removed from further consideration.

4.5. Refractive Index

The dependences of the trans-PFD (Table 8) and cis-PFD (Table 9) refractive index were linear and inversely proportional to temperature (Figure 11). Both were described by Equation (3), and the coefficients are presented in Table 10. In the case of trans-PFD, the dependence of the refractive index was obtained for the 25 to 60 °C range as it is limited by the melting point value. Data on the refractive index value for PFD without specifying the isomeric composition were also presented by Haszeldine [104]. Compared with data reported by Smith [123] (trans-PFD $\Delta n_D^{18\text{ }^\circ\text{C}} = 1.3145_{eq.3}^{exp} - 1.3148^{lit} = -0.0003$ and cis-PFD $\Delta n_D^{18\text{ }^\circ\text{C}} = 1.3180_{Table 9}^{exp} - 1.3179^{lit} = 0.0001$), the values were relatively similar; however, the purity of the investigated samples was relatively low (cis-PFD [123] > 95% mass., trans-PFD [123] > 90% mass.).

The differences in the refractive index of the trans-PFD–cis-PFD, BCH–trans-PFD, and BCH–cis-PFD systems were sufficient to construct calibration curves to determine the composition of the systems on refractive index (Table 11). The dependences of the refractive index on the system's composition (Equation (4)) were composed from the data shown in Figure 12. The coefficients of Equation (4) are listed in Table 12. The acceptable standard uncertainties were: $u(x_i^{nD}) = 0.027$ mole fraction at 25 °C for the trans-PFD–cis-PFD system; $u(x_i^{nD}) = 0.0063$ mole fraction at 15 °C for the BCH–trans-PFD system;

$u(x_i^{np}) = 0.0045$ -mole fraction at 15 °C for the BCH–cis-PFD system. For the BCH–trans-PFD–cis-PFD three-component system, the dependences of the refractive index on composition and temperature were obtained (Table 13), and the behavior of the refractive index isolines at $T = 15$ °C were plotted (Figure 13). In the range of investigating concentration, the dependencies had a linear behavior.

4.6. Density and Liquid Molar Volume

The dependencies of the trans-PFD (Table 14) and cis-PFD (Table 15) density and liquid molar volume were linear and inversely/directly proportional to the temperature, respectively (Figure 14). Both were described by Equations (5) and (6); the equation coefficients are presented in Table 16. In the case of trans-PFD, the dependences of the density and liquid molar volume were obtained for the 25 to 60 °C range as it is limited by the melting point value. Following the example of the viscosity data, comparing the results of the present work with those reported in the literature [90,101,102,104] is difficult due to the absence of the PFD isomeric composition. If the data is compared with that of Varushchenko [145] (trans-PFD $\Delta\rho^{25^\circ\text{C}} = 1.92344_{\text{Table 14}}^{\text{exp}} - 1.9241^{\text{lit}} = -0.00066 \text{ g}\cdot\text{cm}^{-3}$ and cis-PFD $\Delta\rho^{25^\circ\text{C}} = 1.94613_{\text{Table 15}}^{\text{exp}} - 1.9414^{\text{lit}} = 0.00473 \text{ g}\cdot\text{cm}^{-3}$), the values differ in the third digit, but the purity of the investigated samples was unspecified [145].

The dependencies of the density value of the BCH–cis-PFD (Table 17), BCH–trans-PFD (Table 18), and trans-PFD–cis-PFD (Table 19) system's composition were used to calculate the liquid molar volume (Tables 20–22, respectively) and excess molar volume (Tables 23–25, respectively). To create a mathematical model of the excess molar volume versus composition at different temperatures the data were correlated with Equation (9a) equation system (10). The number of parameters in Equation (9a) was sufficient to ensure that the $\sigma(V^E)$ changed negligently with further increases in the value of i ; for the BCH–cis-PFD system, $i = 3$ (Table 26); for the BCH–trans-PFD system, $i = 4$ (Table 27); for the trans-PFD–cis-PFD system, $i = 1$ (Table 28). The temperature parameters of the Redlich–Kister equation according to the Equation (10) system are presented in: Table 29 for the BCH–cis-PFD system, Table 30 for the BCH–trans-PFD system, and Table 31 for the trans-PFD–cis-PFD system. By analogy with Equation (9a), the number of parameters for Equation (10) was sufficient so that the $\sigma(V^E)$ changed negligently with further increases in the i and j values. For the BCH–cis-PFD and BCH–trans-PFD systems, the comparison of experimental (Tables 23 and 24) and calculated by Equation (9a) (Tables 26 and 27) and Equation (10) (Tables 29 and 30) values showed that both models had negligible mutual deviation and described the data within the experimental uncertainty (Figures 15 and 16). The values of excess molar volume in the trans-PFD–cis-PFD system were an order of magnitude lower than in the other two systems under consideration. In the case of the trans-PFD–cis-PFD system, the measured values of the excess molar volume were within the experimental uncertainty (Table 25); both models (Equation (9a) Table 28, Equation (10) Table 31) had mutual deviation but described the data within the experimental uncertainty (Figure 17). Thus, all the correlations could be considered satisfactory.

The dependency of the density value on the BCH–trans-PFD–cis-PFD (Table 32) system's composition was used to calculate the liquid molar volume (Table 33) and excess molar volume (Table 34). The excess molar volume data were correlated with Equation (11) using the temperature-dependent parameters (Tables 29–31). The data calculated by the Kohler Equation (11) on the excess molar volume for the BCH–trans-PFD–cis-PFD system are listed in Table 35. From the comparison of Tables 34 and 35 data, it can be concluded that the model describes the experimental data within the experimental standard uncertainty. The curves of the isolines of the excess molar volume in the BCH–trans-PFD–cis-PFD system are shown in Figure 18. The highest values of excess molar volume corresponded to the composition of the BCH–cis-PFD close to the equimolar.

5. Conclusions

The obtained experimental data partially supplement and, in many aspects, extend the information presented in the literature. First, the new experimental data provide background information and a starting point for further research. For example, the obtained data are necessary for engineering calculations of individual apparatuses (calculation of mass transfer coefficients, hydrodynamic properties, heat exchange devices, Rayleigh, Prandtl, Nusselt, and Reynolds numbers) and the process in general (engineering analysis or mathematical modeling with modern software complexes, such as Aspen Plus and others). In addition, these data may interest researchers of both allied and very distant field sciences.

Supplementary Materials: The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/pr11113208/s1>, ^{19}F NMR, FTIR and GC-MS original files for cis-perfluorodecalin and trans-perfluorodecalin.

Author Contributions: Conceptualization, E.V.L. and A.V.P.; methodology, E.V.L. and A.V.P.; validation, E.V.L. and A.V.P.; formal analysis, E.V.L. and A.V.P.; investigation, E.V.L., A.V.P. and A.V.K.; writing—original draft preparation, A.V.P.; writing—review and editing, E.V.L., A.V.P., N.N.K., Y.A.Z. and A.A.V.; visualization, A.V.P.; supervision, A.V.P., E.V.L. and A.A.V.; project administration, A.V.P., E.V.L. and N.N.K.; funding acquisition, A.A.V., N.N.K. and Y.A.Z. All authors have read and agreed to the published version of the manuscript.

Funding: This study was financially supported by the Russian Science Foundation, project no. 22-29-00791, <https://rscf.ru/en/project/22-29-00791/> (access date 9 November 2023).

Data Availability Statement: Data is contained within the article or Supplementary Materials.

Acknowledgments: NMR and chromatography–mass spectrometry data were obtained using the equipment of the JRC PMR IGIC RAS.

Conflicts of Interest: The authors declare no competing financial interests.

Nomenclature

Reductions

| | |
|------|---|
| BCH | perfluoro(butyl)cyclohexane) |
| DSC | differential scanning calorimetry |
| FTIR | Fourier transform infrared spectrum |
| GC | gas chromatography |
| MBCN | perfluoro(7-methylbicyclo[4.3.0]nonane) |
| NMR | nuclear magnetic resonance |
| PFD | perfluorodecalin |

Symbols

| | |
|-----------------------------------|---|
| $A_i^{n_D}, B_i^{n_D}$ | coefficients of Equation (3) |
| A_i^p, B_i^p, C_i^p | coefficients of Antoine equation |
| A_i^p, B_i^p | coefficients of Equation (6) |
| $a_0^{n_D}, a_1^{n_D}, a_2^{n_D}$ | coefficients of Equation (4). |
| a_i | Redlich-Kister parameters |
| b_j | parameters of the Equation (10b) |
| ΔC_p | heat capacity change, $\text{J}\cdot\text{g}^{-1}\cdot\text{K}^{-1}$ |
| d | number of compositions studied |
| E_a | apparent activation energy for the viscous flow, $\text{J}\cdot\text{mol}^{-1}$ |
| f | function |
| H | enthalpy, $\text{J}\cdot\text{g}^{-1}$ |
| M | molecular weight, $\text{g}\cdot\text{mole}^{-1}$ |
| m | sample weight, g |
| \tilde{n} | number of terms used in the regression |
| n_D | refractive index |
| P | pressure, kPa |
| $R = 8.314$ | molar gas constant, $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ |

Table A2. Dependences of the standard deviation values of liquid molar volume $u(V_M)$ on perfluoro(butylcyclohexane) (1)–trans-perfluorodecalin (2) system composition x_i at temperature T .

| x_1 | $T/^\circ\text{C}$ | | | | | | | |
|---------|---|-------|-------|-------|-------|-------|-------|-------|
| | 25 | 30 | 35 | 40 | 45 | 50 | 55 | 60 |
| | $u(V_M)/\text{cm}^{-3}\cdot\text{mol}^{-1}$ | | | | | | | |
| 0 | 0.012 | 0.013 | 0.013 | 0.013 | 0.013 | 0.013 | 0.013 | 0.014 |
| 0.10688 | 0.017 | 0.017 | 0.017 | 0.017 | 0.017 | 0.017 | 0.018 | 0.018 |
| 0.19419 | 0.017 | 0.017 | 0.017 | 0.017 | 0.017 | 0.018 | 0.018 | 0.018 |
| 0.29614 | 0.019 | 0.020 | 0.020 | 0.020 | 0.020 | 0.020 | 0.020 | 0.021 |
| 0.40516 | 0.020 | 0.020 | 0.020 | 0.020 | 0.020 | 0.020 | 0.021 | 0.021 |
| 0.49698 | 0.020 | 0.020 | 0.020 | 0.020 | 0.020 | 0.021 | 0.021 | 0.021 |
| 0.59993 | 0.020 | 0.020 | 0.020 | 0.020 | 0.021 | 0.021 | 0.021 | 0.021 |
| 0.69763 | 0.023 | 0.023 | 0.023 | 0.023 | 0.024 | 0.024 | 0.024 | 0.024 |
| 0.80471 | 0.023 | 0.023 | 0.023 | 0.024 | 0.024 | 0.024 | 0.024 | 0.024 |
| 0.89712 | 0.026 | 0.026 | 0.026 | 0.027 | 0.027 | 0.027 | 0.027 | 0.028 |
| 1 | 0.014 | 0.015 | 0.015 | 0.015 | 0.015 | 0.015 | 0.015 | 0.016 |

Table A3. Dependences of the standard deviation values of liquid molar volume $u(V_M)$ on trans-perfluorodecalin (1)–cis-perfluorodecalin (2) system composition x_i at temperature T .

| x_1 | $T/^\circ\text{C}$ | | | | | | | |
|---------|---|-------|-------|-------|-------|-------|-------|-------|
| | 25 | 30 | 35 | 40 | 45 | 50 | 55 | 60 |
| | $u(V_M)/\text{cm}^{-3}\cdot\text{mol}^{-1}$ | | | | | | | |
| 0 | 0.012 | 0.012 | 0.012 | 0.013 | 0.013 | 0.013 | 0.013 | 0.013 |
| 0.10198 | 0.012 | 0.012 | 0.013 | 0.013 | 0.013 | 0.013 | 0.013 | 0.013 |
| 0.19411 | 0.012 | 0.012 | 0.013 | 0.013 | 0.013 | 0.013 | 0.013 | 0.013 |
| 0.30439 | 0.012 | 0.012 | 0.013 | 0.013 | 0.013 | 0.013 | 0.013 | 0.013 |
| 0.41417 | 0.012 | 0.012 | 0.013 | 0.013 | 0.013 | 0.013 | 0.013 | 0.013 |
| 0.49848 | 0.012 | 0.012 | 0.013 | 0.013 | 0.013 | 0.013 | 0.013 | 0.013 |
| 0.60085 | 0.012 | 0.013 | 0.013 | 0.013 | 0.013 | 0.013 | 0.013 | 0.013 |
| 0.70172 | 0.012 | 0.013 | 0.013 | 0.013 | 0.013 | 0.013 | 0.013 | 0.013 |
| 0.80539 | 0.012 | 0.013 | 0.013 | 0.013 | 0.013 | 0.013 | 0.013 | 0.014 |
| 0.90273 | 0.012 | 0.013 | 0.013 | 0.013 | 0.013 | 0.013 | 0.013 | 0.014 |
| 1 | 0.012 | 0.013 | 0.013 | 0.013 | 0.013 | 0.013 | 0.013 | 0.014 |

Table A4. Dependences of the standard deviation values of excess molar volume $u(V^E)$ on perfluoro(butylcyclohexane) (1)–cis-perfluorodecalin (2) system composition x_i at temperature T .

| x_1 | $T/^\circ\text{C}$ | | | | | | | | | |
|---------|---|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| | 15 | 20 | 25 | 30 | 35 | 40 | 45 | 50 | 55 | 60 |
| | $u(V^E)/\text{cm}^{-3}\cdot\text{mol}^{-1}$ | | | | | | | | | |
| 0.10343 | 0.030 | 0.030 | 0.030 | 0.031 | 0.031 | 0.031 | 0.031 | 0.031 | 0.032 | 0.032 |
| 0.17164 | 0.019 | 0.019 | 0.019 | 0.020 | 0.020 | 0.020 | 0.020 | 0.020 | 0.020 | 0.021 |
| 0.28538 | 0.030 | 0.030 | 0.030 | 0.030 | 0.030 | 0.030 | 0.031 | 0.031 | 0.031 | 0.031 |
| 0.31744 | 0.021 | 0.022 | 0.022 | 0.022 | 0.022 | 0.022 | 0.023 | 0.023 | 0.024 | 0.024 |
| 0.35826 | 0.025 | 0.025 | 0.026 | 0.026 | 0.026 | 0.027 | 0.027 | 0.027 | 0.027 | 0.028 |
| 0.37933 | 0.025 | 0.025 | 0.026 | 0.026 | 0.026 | 0.027 | 0.027 | 0.027 | 0.027 | 0.028 |
| 0.39919 | 0.025 | 0.025 | 0.026 | 0.026 | 0.026 | 0.027 | 0.027 | 0.027 | 0.027 | 0.028 |
| 0.44022 | 0.025 | 0.025 | 0.026 | 0.026 | 0.026 | 0.027 | 0.027 | 0.027 | 0.028 | 0.028 |
| 0.50224 | 0.025 | 0.026 | 0.026 | 0.026 | 0.027 | 0.027 | 0.027 | 0.027 | 0.028 | 0.028 |
| 0.60547 | 0.026 | 0.026 | 0.027 | 0.027 | 0.027 | 0.027 | 0.027 | 0.028 | 0.028 | 0.028 |
| 0.69350 | 0.030 | 0.031 | 0.031 | 0.031 | 0.031 | 0.031 | 0.031 | 0.032 | 0.032 | 0.033 |
| 0.80202 | 0.031 | 0.031 | 0.031 | 0.032 | 0.032 | 0.032 | 0.033 | 0.033 | 0.033 | 0.033 |
| 0.88860 | 0.032 | 0.032 | 0.032 | 0.032 | 0.032 | 0.033 | 0.033 | 0.033 | 0.033 | 0.034 |

Table A5. Dependences of the standard deviation values of excess molar volume $u(V^E)$ on perfluoro(butylcyclohexane) (1)–trans-perfluorodecalin (2) system composition x_i at temperature T .

| x_1 | $T/^\circ\text{C}$ | | | | | | | |
|---------|---|-------|-------|-------|-------|-------|-------|-------|
| | 25 | 30 | 35 | 40 | 45 | 50 | 55 | 60 |
| | $u(V^E)/\text{cm}^{-3}\cdot\text{mol}^{-1}$ | | | | | | | |
| 0.10688 | 0.023 | 0.023 | 0.023 | 0.023 | 0.024 | 0.024 | 0.024 | 0.024 |
| 0.19419 | 0.022 | 0.023 | 0.023 | 0.023 | 0.023 | 0.024 | 0.024 | 0.024 |
| 0.29614 | 0.026 | 0.026 | 0.026 | 0.027 | 0.027 | 0.027 | 0.027 | 0.028 |
| 0.40516 | 0.026 | 0.026 | 0.026 | 0.027 | 0.027 | 0.027 | 0.027 | 0.028 |
| 0.49698 | 0.026 | 0.026 | 0.027 | 0.027 | 0.027 | 0.027 | 0.028 | 0.028 |
| 0.59993 | 0.026 | 0.027 | 0.027 | 0.027 | 0.027 | 0.028 | 0.028 | 0.028 |
| 0.69763 | 0.031 | 0.031 | 0.031 | 0.032 | 0.032 | 0.032 | 0.033 | 0.033 |
| 0.80471 | 0.031 | 0.032 | 0.032 | 0.032 | 0.033 | 0.033 | 0.033 | 0.033 |
| 0.89712 | 0.036 | 0.037 | 0.037 | 0.037 | 0.037 | 0.038 | 0.038 | 0.038 |

Table A6. Dependences of the standard deviation values of excess molar volume $u(V^E)$ on trans-perfluorodecalin (1)–cis-perfluorodecalin (2) system composition x_i at temperature T .

| x_1 | $T/^\circ\text{C}$ | | | | | | | |
|---------|---|-------|-------|-------|-------|-------|-------|-------|
| | 25 | 30 | 35 | 40 | 45 | 50 | 55 | 60 |
| | $u(V^E)/\text{cm}^{-3}\cdot\text{mol}^{-1}$ | | | | | | | |
| 0.10198 | 0.022 | 0.022 | 0.023 | 0.023 | 0.023 | 0.023 | 0.024 | 0.024 |
| 0.19411 | 0.021 | 0.021 | 0.022 | 0.023 | 0.023 | 0.023 | 0.023 | 0.023 |
| 0.30439 | 0.021 | 0.021 | 0.021 | 0.022 | 0.022 | 0.022 | 0.022 | 0.022 |
| 0.41417 | 0.020 | 0.020 | 0.021 | 0.021 | 0.021 | 0.021 | 0.021 | 0.021 |
| 0.49848 | 0.020 | 0.020 | 0.021 | 0.021 | 0.021 | 0.021 | 0.021 | 0.022 |
| 0.60085 | 0.020 | 0.021 | 0.021 | 0.021 | 0.021 | 0.021 | 0.021 | 0.022 |
| 0.70172 | 0.021 | 0.022 | 0.022 | 0.022 | 0.022 | 0.022 | 0.022 | 0.022 |
| 0.80539 | 0.021 | 0.022 | 0.022 | 0.022 | 0.023 | 0.023 | 0.023 | 0.024 |
| 0.90273 | 0.022 | 0.024 | 0.024 | 0.024 | 0.024 | 0.024 | 0.024 | 0.025 |

Table A7. Standard deviations σ (Equation (9b)) between experimental (Table 23) and calculated by Equation (10) (Table 29) data for the perfluoro(butylcyclohexane) (1)–trans-perfluorodecalin (2) system.

| $T/^\circ\text{C}$ | $\sigma(V^E)/\text{cm}^{-3}\cdot\text{mol}^{-1}$ |
|--------------------|--|
| 15 | 0.023 |
| 20 | 0.020 |
| 25 | 0.020 |
| 30 | 0.019 |
| 35 | 0.019 |
| 40 | 0.018 |
| 45 | 0.018 |
| 50 | 0.021 |
| 55 | 0.019 |
| 60 | 0.020 |

Table A8. Standard deviations σ (Equation (9b)) between experimental (Table 24) and calculated by Equation (10) (Table 30) data for the perfluoro(butylcyclohexane) (1)–cis-perfluorodecalin (2) system.

| $T/^\circ\text{C}$ | $\sigma(V^E)/\text{cm}^{-3}\cdot\text{mol}^{-1}$ |
|--------------------|--|
| 25 | 0.019 |
| 30 | 0.015 |
| 35 | 0.013 |
| 40 | 0.012 |
| 45 | 0.012 |
| 50 | 0.013 |
| 55 | 0.013 |
| 60 | 0.011 |

Table A9. Standard deviations σ (Equation (9b)) between experimental (Table 25) and calculated by Equation (10) (Table 31) data for the trans-perfluorodecalin (1)–cis-perfluorodecalin (2) system.

| $T/^\circ\text{C}$ | $\sigma(V^E)/\text{cm}^{-3}\cdot\text{mol}^{-1}$ |
|--------------------|--|
| 25 | 0.010 |
| 30 | 0.009 |
| 35 | 0.010 |
| 40 | 0.011 |
| 45 | 0.020 |
| 50 | 0.010 |
| 55 | 0.008 |
| 60 | 0.007 |

Table A10. Dependences of the standard deviation values of liquid molar volume $u(V_M)$ on perfluoro(butylcyclohexane) (1)–trans-perfluorodecalin (2)–cis-perfluorodecalin (3) system composition x_i at temperature T .

| x_1 | x_2 | x_3 | $T/^\circ\text{C}$ | | | | | | | |
|---|---------|---------|--------------------|-------|-------|-------|-------|-------|-------|-------|
| | | | 25 | 30 | 35 | 40 | 45 | 50 | 55 | 60 |
| $u(V_M)/\text{cm}^{-3}\cdot\text{mol}^{-1}$ | | | | | | | | | | |
| 0.57402 | 0.21988 | 0.20610 | 0.022 | 0.022 | 0.023 | 0.023 | 0.023 | 0.023 | 0.023 | 0.024 |
| 0.17479 | 0.19519 | 0.63002 | 0.021 | 0.021 | 0.022 | 0.022 | 0.022 | 0.022 | 0.022 | 0.023 |
| 0.17937 | 0.63244 | 0.18819 | 0.021 | 0.021 | 0.021 | 0.022 | 0.022 | 0.022 | 0.022 | 0.022 |
| 0.18870 | 0.39863 | 0.41267 | 0.020 | 0.020 | 0.020 | 0.020 | 0.021 | 0.021 | 0.021 | 0.021 |
| 0.36974 | 0.40875 | 0.22151 | 0.020 | 0.021 | 0.021 | 0.021 | 0.021 | 0.021 | 0.022 | 0.022 |
| 0.37885 | 0.22255 | 0.39860 | 0.020 | 0.020 | 0.021 | 0.021 | 0.021 | 0.021 | 0.021 | 0.022 |

Table A11. Dependences of the standard deviation values of excess molar volume $u(V^E)$ on perfluoro(butylcyclohexane) (1)–trans-perfluorodecalin (2)–cis-perfluorodecalin (3) system composition x_i at temperature T .

| x_1 | x_2 | x_3 | $T/^\circ\text{C}$ | | | | | | | |
|---|---------|---------|--------------------|-------|-------|-------|-------|-------|-------|-------|
| | | | 25 | 30 | 35 | 40 | 45 | 50 | 55 | 60 |
| $u(V^E)/\text{cm}^{-3}\cdot\text{mol}^{-1}$ | | | | | | | | | | |
| 0.57402 | 0.21988 | 0.20610 | 0.183 | 0.184 | 0.185 | 0.186 | 0.186 | 0.187 | 0.187 | 0.189 |
| 0.17479 | 0.19519 | 0.63002 | 0.181 | 0.182 | 0.182 | 0.184 | 0.184 | 0.184 | 0.185 | 0.186 |
| 0.17937 | 0.63244 | 0.18819 | 0.179 | 0.181 | 0.181 | 0.182 | 0.182 | 0.183 | 0.183 | 0.185 |
| 0.18870 | 0.39863 | 0.41267 | 0.173 | 0.174 | 0.174 | 0.175 | 0.176 | 0.176 | 0.177 | 0.178 |
| 0.36974 | 0.40875 | 0.22151 | 0.174 | 0.176 | 0.176 | 0.177 | 0.177 | 0.177 | 0.178 | 0.180 |
| 0.37885 | 0.22255 | 0.39860 | 0.173 | 0.174 | 0.175 | 0.176 | 0.176 | 0.177 | 0.177 | 0.178 |

Table A12. Standard deviations σ (Equation (9b)) between experimental (Table 34) and calculated by Equation (11) (Table 35) data for the perfluoro(butylcyclohexane) (1)–trans-perfluorodecalin (2) system–cis-perfluorodecalin (3) system.

| $T/^\circ\text{C}$ | $\sigma(V^E)/\text{cm}^{-3}\cdot\text{mol}^{-1}$ |
|--------------------|--|
| 25 | 0.047 |
| 30 | 0.043 |
| 35 | 0.041 |
| 40 | 0.040 |
| 45 | 0.050 |
| 50 | 0.043 |
| 55 | 0.041 |
| 60 | 0.041 |

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