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BRIEF COMMUNICATIONS

Physicochemical Properties of 1,2-Epoxycyclopentane

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Abstract—Temperature dependences of density, viscosity, and saturated vapor pressure of 1,2-epoxycyclopentane were studied and approximated by interpolation equations. Its refraction index and chromato-mass-spectroscopy data are given.

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An effective direction of using cyclopentene extracted from the C_5-fraction of gasoline pyrolysis is the synthesis of 1,2-epoxycyclopentane and oxygen-containing compounds on its basis. Alicyclic epoxides and their derivatives are applied to obtain polymeric materials possessing a high heat resistance, good insulating properties, and enhanced mechanical strength. They are widely used in production of glues, varnishes, enamels and in the synthesis of pharmaceutical and antibacterial products [1].

The information on the main physicochemical properties of 1,2-epoxycyclopentane is absent from the literature. In the present work such properties are described in detail for the first time.

EXPERIMENTAL

1,2-Epoxycyclopentane was synthesized by the liquid-phase oxidation of cyclopentene by isopropyl benzene hydroperoxide and was isolated by rectification with the yield of 99.5 wt % [2]. The structure and purity of 1,2-epoxycyclopentane were confirmed by the IR and chromato-mass-spectroscopy methods. The presence of the epoxy group in the IR spectrum is characterized by the bands of stretching vibrations at 3026.29, 1299.38, and 921.77 cm^{-1} and a band at 839.78 cm^{-1}. A band at 2956.56 cm^{-1} corresponds to the -CH_2- groups of the ring.

The electron impact spectra were recorded on a GC/MS Perkin-Elmer Clarus 500 instrument. The mass-spectrometer was quadrupole, ionization energy 70 eV. The mass-spectrometer was adjusted by perfluorobutylamine. An Elite 5MS gas chromatograph column was of a capillary type, the length of 30 m, the diameter of 0.25 mm, and the phase width of 0.25 μm. A chromatogram and a mass spectrum of the compound under study are

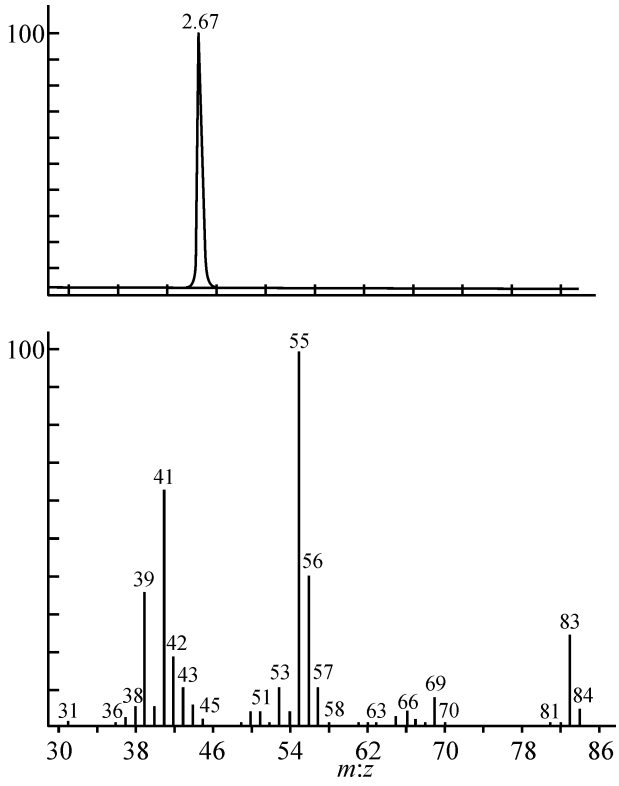

Fig. 1. Chromatogram and mass spectrum of 1.2-epoxycyclopentane.

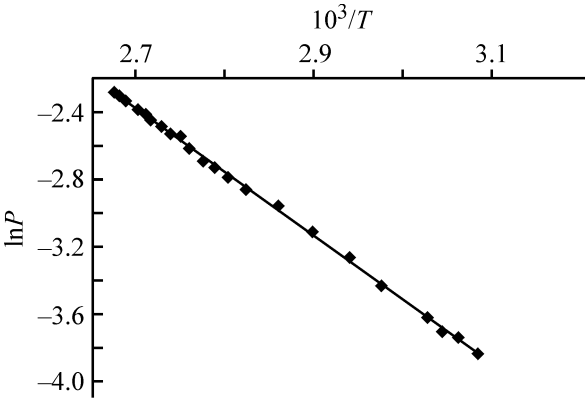

Fig. 2. Logarithmic dependence of saturated vapor pressure P (MPa) of 1.2-epoxycyclopentane on inverse temperature T (K). Points: experimental values, line: calculated data ($R^2 = 0.981$).

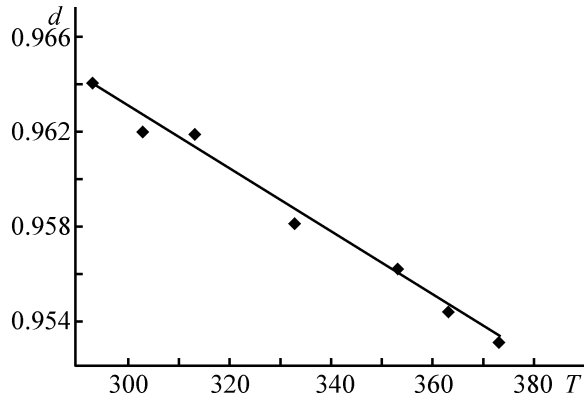

Fig. 3. Dependence of density d (g cm^{-3}) of 1.2-epoxycyclopentane on temperature T (K). Points: experimental values, line: calculated data ($R^2 = 0.973$).

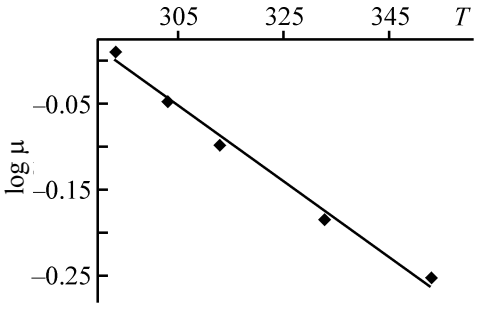

Fig. 4. Logarithmic dependence of viscosity μ (MPa s) of 1,2-epoxycyclopentane on temperature T (K). Points: experimental values, line: calculated data ($R^2 = 0.985$).

presented in Fig. 1, which shows that the retention time of 1,2-epoxycyclopentane is 2.67 min.

1,2-Epoxycyclopentane is a colorless transparent liquid with a specific odor, it is readily soluble in ethanol, acetone, aromatic hydrocarbons, and partially soluble in water.

Saturated vapor pressure P, density d, and viscosity μ of 1,2-epoxycyclopentane at various temperature

T, °C	P[a], Mpa	d, g cm^{-3}	μ, MPa s
20	–	0.9640	1.0148
25	–	0.9633	0.9546
30		0.9627	0.8999
35	–	0.9620	0.8499
40	–	0.9613	0.8042
45	–	0.9606	0.7622
50	0.0197	0.9600	0.7236
55	0.0239	0.9593	0.6881
60	0.0286	0.9586	0.6553
65	0.0341	0.9580	0.6250
70	0.0404	0.9573	0.5969
75	0.0475	0.9566	0.5708
80	0.0555	0.9560	0.5466
85	0.0644	0.9553	0.5240
90	0.0745	0.9546	0.5029
95	0.0856	0.9539	0.4832
100	0.0979	0.9533	0.4648

[a] No measurements were carried out in the temperature range 20–50°C.

Refraction index of 1,2-epoxycyclopentane was determined on an IRF-22 refractometer, $n_d^{20} = 1.4339$, published $n_d^{20} = 1.4336$.

The temperature dependence of the saturated vapor pressure of 1,2-epoxycyclopentane was determined using a Washbourn ebulliometer, introducing corrections for exterior pressure. The experimental data were approximated by the Antoine equation [4]

$$\ln P = A - \frac{B}{C+T},$$

where A, B, and C are coefficients of the Antoine equation; T is temperature (K).

In the temperatures range of 50-100°C the coefficients for 1,2-epoxycyclopentane were: $A = 5.2289$, $B = 2158.37$, and $C = -87.221$. The relative error of calculated values did not exceed 3%. The dependence of the logarithm of 1.2-epoxycyclopentane vapor pressure on inverse temperature is of the rectilinear shape (Fig. 2).

Density of 1,2-epoxycyclopentane was determined using a standard volumetric flask of the 2 cm^3 volume [5]. To eliminate accidental errors, we carried out several

parallel measurements and calculated average values, provided that discrepancy between measurements does not exceed 0.008 g. The temperature dependence of the 1,2-epoxycyclopentane density in the range 20–100°C is described by the linear equation (Fig. 3)

$$d_4^T = -1.34 \cdot 10^{-4} T + 1.0033.$$

The relative error of the calculated values does not exceed 0.5%.

We measured 1,2-epoxycyclopentane viscosity using a VPZh-2 capillary viscometer with a capillary diameter of 0.73 mm [6].

The temperature dependence of viscosity is adequately described by the straight-line equation (Fig. 4)

$$\log \mu = B\left(\frac{1}{T} - \frac{1}{T_0}\right),$$

where B and T_0 are parameters of the equation connected with the compound structure.

The values of these parameters for 1,2-epoxycyclopentane found on the experimental basis are: $B = 463.22$ and $T_0 = 294.18$. The relative error of the calculated values does not exceed 1.5%.

The data on the physical properties of 1,2-epoxycyclopentane calculated by the obtained equations for various temperatures are presented in the table.

CONCLUSIONS

1,2-Epoxycyclopentane containing no less than 99.5% of the main substance was synthesized by the hydroperoxide oxidation of cyclopentene, and its physicochemical properties were studied. On the basis of the experimental data interpolational equations for the temperature dependences of density, viscosity, and saturated vapor pressure of 1,2-epoxycyclopentane were obtained.

REFERENCES

1. Kas'yan, L.I., Seferova, M.F., and Okovityi, S.I., *Atsiklicheskie epoksidnye soedineniya: Metody sinteza* (Acyclic Epoxyde Compounds: Methods of Synthesis), Dnepropetrovsk: Dnepropetrovsk State University, 2003, 2-nd ed.
2. Meshechkina, A.E., Mel'nik, L.V., Rybina, G.V., et al., *Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol*., 2008, vol. 51, no. 8, pp. 39-42.
3. *Aldrich Catalog: Handbook of Fine Chemicals. Supplement*, Milwauke: Aldrich Chemical Company, 1988.
4. Kogan, V.B., Fridman, V.M., and Kafarov, V.V., *Ravnovesie mezhdu zhidkost'yu i parom* (Vapor-Liquid Equilibrium), Leningrad: Nauka, 1966, vol. 1.
5. *Praktikum po fizicheskoi khimii* (Laboratory Manual on Physical Chemistry), Gorbachev, S.V., Ed., Moscow: Vysshaya shkola, 1974.
6. Pisarenko, V.V. and Zakharov, L.S., *Osnovy tekhnicheskogo analiza* (Fundamentals of Technical Analysis), Moscow: Vysshaya shkola, 1972.