



Scientific article

UDC 678.7:544.3

DOI: 10.52957/27821900\_2022\_04\_71

## THE CALCULATION OF SOLUBILITY PARAMETERS FOR NITRILE-BUTADIENE RUBBERS BY THE GROUP ADDITIVITY METHOD

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### Keywords:

butadiene nitrile rubbers, solubility parameters, group additivity method

**Abstract.** Butadiene Nitrile Rubber (BNR) is a special purpose elastomer with an increased resistance to aliphatic hydrocarbon solvents, oils, and fuels. Depending on the monomer ratio of the butadiene-nitrile copolymers, their compatibility with different types of solvents and plasticisers varies considerably. In addition, BNRs with carboxyl, hydroxyl and hydrogenated BNRs are industrially available.

The purpose of the study was to calculate the solubility parameters of different compositions of BNRs copolymers, hydrogenated BNRs, and rubbers with hydroxyl and carboxyl groups. We calculated the increments of the functional groups of copolymers under study and the molecular attraction by the Small constants. The calculations based on the processing of reference data on the enthalpies of evaporation and molar volume of aliphatic and aromatic hydrocarbons, nitriles, acids, alcohols, and esters. Also we used the increments obtained to calculate three dimensional solubility parameters of the copolymers as well as the dependencies of the change in Gibbs free energy at mixing on the solvent volume fraction for the two types of solvents.

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For citation:

Solovyev, M.E., Kablov, V.F., Solovyova, O.Yu., Shulmin, S.N. & Orlova, E.N. (2022) The calculation of solubility parameters of butadiene nitrile rubbers by the group additivity method, *From Chemistry Towards Technology Step-By-Step*, 3(4), pp. 71-79 [online]. Available at: <http://chemintech.ru/index.php/tor/2022-3-4>

### Introduction

Butadiene-nitrile copolymers are one of the oldest special purpose rubbers [1, 2]. Nowadays the most important area of their application is the production of rubber products with improved resistance to aliphatic hydrocarbons, including oils and various fuels. The integration of the additional links containing carboxylic and hydroxyl groups into the copolymer composition extends the range of special properties of the rubbers and improves the adhesion to metals, providing the possibility of their vulcanisation with metal oxides [3-7]. Depending on the synthesis method, the functional groups can be distributed statistically along the polymer chain



or arranged at its ends (butadiene nitrile copolymers with end carboxyl groups - CTBN and end hydroxyl groups - HTBN) [8-11]. Nowadays, hydrogenated butadiene nitrile rubbers containing no double bonds and with improved resistance to heat aging are industrially produced [12, 13].

In order to predict the solvent compatibility of the chemically complex copolymers, it is necessary to have techniques to calculate two- and three-dimensional parameters of their solubility. The classical method used to calculate the solubility parameters of polymers and low molecular weight solvents is the group additivity method [14]. Organic chemistry traditionally uses this method to calculate the physical and physicochemical properties of compounds. This method is still actual one [17], although there are the other ones based on more complex molecular structure descriptors [15, 16]. In our study we use this particular method because the calculation of enthalpies of evaporation and compounds molar volumes of individual functional groups have a definite physical meaning that allows their use at interpretation of data related to intermolecular interactions of different classes of organic compounds [18-20].

The purpose of this study was to calculate the increments of the functional groups, copolymers, and solvents considered in the enthalpy of evaporation, molar volume, and molecular attraction of the Small constants in order to calculate the solubility parameters of the compounds under study.

### Main body

The monograph [14] contains the increments of many functional groups in thermodynamic functions calculated by different authors, which are used not only to define the solubility parameters of polymers and low molecular weight fluids, but also to evaluate their compatibility. The numerical values of the increments of the same functional groups given in the works of different authors are quite different. The reason is the rare presence of the strict additivity in the influence of individual functional groups [17]. Therefore, increasing of the chemical compounds quantity for calculating the increments of functional groups causes decreasing of the thermodynamic functions predictions accuracy, based on the additive approach. In this study we calculated increments of compounds functional groups with the relative chemical structure of copolymers and plasticizers under study. We used the experimental data on enthalpy of evaporation and molar volume of compounds [21, 22] as well as NIST databases on thermodynamic properties of compounds [23] as an initial set for compiling the training sample.

The group additivity method can be applied for isolation of the individual atomic groups common to compounds of different classes, and show the physical property of a compound  $Y$  as a linear function of the number of groups, relative to the number of moles:

$$Y = \sum_{i=1}^N B_i n_i, \quad (1)$$

where  $B_i$  is the increment of the corresponding group,  $n_i$  is the number of groups of each type in a particular chemical structure,  $N$  is the number of group types.

The use of the atomic groups, rather than the individual atoms, as descriptors of the molecular structure is based on the structural classification of the organic compounds, according to which compounds with the same types of the atomic groups (aldehydes, ketones, alcohols,



acids, etc.) are characterised by common features of the chemical and physicochemical properties. As the different atomic groups and spatial isomerism influence each other, therefore the simple linear model (1) is a good initial approximation.

The advantage of the linear model is also the simplicity of parameter assessment  $B_i$ . In terms of experimental-statistical methods [24], equation (1) is a linear regression equation  $n_i$  containing the independent variables and the regression parameters.

We consider the training sample including  $M$  compounds with the experimentally determined value of the property  $y_j, j = 1 \dots M$  to calculate the coefficients of the  $B_i$  regression equation (1). For each  $j$ -th connection we know the parameters of its structure  $x_{ji}, i = 1 \dots N$ , the whole set of which we will denote by the matrix  $X$ . To find the vector of regression equation coefficients, it is necessary to minimise a function of the type

$$W = (y - XB)^T(y - XB) \quad (2)$$

for the variables  $B_i$ .

By the necessary condition of extremum

$$\frac{\partial W}{\partial B} = 0 \quad (3)$$

it is easy to obtain the well-known formula of regression analysis to calculate the least-squares estimates of the regression coefficients:

$$B = (X^T X)^{-1} X^T y. \quad (4)$$

Calculation by this formula can be performed using automation software that supports the linear algebra operations [24]. We use the function that implements this formula as the integrated one for the Libre Office Calc Programme.

Based on a sample of enthalpies of evaporation under standard conditions ( $dH^0$ ) and molar volumes ( $V_m$ ) of compounds from classes of alkanes, alkenes, arenes, nitriles, acids, alcohols, esters, and chloroalkanes using formula (4), we calculate the increments of atomic groups in these physical properties as well as increments in molecular attraction by the Small constant [25] (Table 1):

$$F = (E_{coh} V_m)^{1/2}, \quad (5)$$

where  $E_{coh} = dH^0 - RT$  is the cohesion energy.

**Table 1.** Atomic group increments calculated from a sample of 142 compounds

Atomic group	$dH^0$ , kJ/mol	$V_m$ , m <sup>3</sup> /mol·10 <sup>6</sup>	$F$ , (MJ/mol <sup>3</sup> ) <sup>1/2</sup> /mol
-C=C-	10.24	26.69	504.08
-OH	30.49	9.23	866.27
-CN	22.12	22.27	786.45
-COOH	44.64	28.14	1323.24
-COOCH <sub>3</sub>	17.13	21.72	676.62
-C <sub>6</sub> H <sub>5</sub>	35.67	93.88	1771.68
-Cl	12.17	24.05	533.91
-CH <sub>3</sub>	5.54	27.71	376.45
-CH <sub>2</sub> -	4.98	17.28	290.9
>CH-	3.29	10.15	178.56



We assessed the statistical validity of the regression models using the value of the determination coefficient

$$R^2 = 1 - \frac{\sum(y_i - \hat{y}_i)^2}{\sum(y_i - \bar{y})^2}, \quad (6)$$

where  $\hat{y}_i$  - is the response value calculated by the regression equation,  $\bar{y}$  - is the average of the sample response values.

A value close  $R^2$  to unity indicates the high reliability of the linear approximation.

Also we assessed the accuracy of the property prediction by the confidence interval value of the predicted response value

$$\Delta\hat{y} = \sqrt{S_{ad}^2 T_{inv}(0.05, M - N)}, \quad (7)$$

where  $S_{ad}^2 = \frac{1}{M-N} \sum(y_i - \hat{y}_i)^2$  is the variance of the model adequacy,  $T_{inv}(0.05, M - N)$  is the quantile of the Student distribution.

The relative error of the property prediction was estimated by dividing the confidence interval of the response prediction by its sample mean.

The statistical analysis of the regression models indicates a high reliability of the approximation for all properties studied (Table 2). The relative error in the prediction of  $F$  is smaller than for  $dH^0$  and  $V_m$ . Therefore, we can conclude that the calculation of the solubility  $\delta$  parameters by the Small molecular attraction constants

$$\delta = \frac{F}{V_m} \quad (8)$$

is more accurate than the cohesion energy density calculation

$$\delta = \left( \frac{E_{coh}}{V_m} \right)^{\frac{1}{2}}. \quad (9)$$

**Table 2.** The results of the statistical analysis of linear models (1)

Statistical parameter	$dH^0$	$V_m$	$F$	Fedors, $dH^0$	Fedors, $V_m$
$R^2$	0.993	0.986	0.994	0.929	0.909
Confidence interval	2.81	12.96	135.68	9.10	33.55
Relative error	3.01%	4.41%	2.70%	9.74%	11.42%

The last two columns of Table 2 show the results of the statistical analysis of the evaporation enthalpy and free volume models calculated by the increments obtained in Fedors [26] and in [14]. These increments are calculated by a sample including a much larger number of classes of compounds, and therefore containing a larger number of the different atomic groups. We can assume that expanding of the set of atomic groups in the sample increases its representativeness. However, by Table 2, this expanding actually causes the predictive accuracy degradation of the model compared to a model with fewer parameters. It is a consequence of the interaction of different types of atomic groups, appearing in samples with a large number of compound classes. We can obtain the same result by analysing the incremental values obtained by Fedors. In particular, the molar volume increments for some atomic groups in the Fedors database have negative values. This contradicts their physical values and indicates that the estimates



of these coefficients are correlated with the other coefficients in the equation. Under these conditions, it is not appropriate to use the linear model (1) and the equation should be firstly supplemented with terms considering the interaction of the variables. Also, the increment of the carboxylic group in the cohesion energy density of Fedors is smaller than that of the hydroxyl group, and almost equal to the increment of the nitrile group. All above contradicts our data based on samples with a small set of compound types [27, 28] as well as the quantum-chemical estimates of the intermolecular interaction energy of these atomic groups [28].

Since the relative error in calculating the molecular attraction of the Small constants is smaller than in calculating the enthalpy of evaporation, the solubility parameters of polymers and plasticisers were calculated by the increments of the molecular attraction constants  $F_i$

$$\delta = \frac{1}{V_m} \sum F_i n_i. \quad (10)$$

When calculating the two- and three-dimensional solubility parameters the increments  $F_i$  were divided, respectively, into two or three groups, relating the increments of  $-\text{CH}_3$ ,  $-\text{CH}_2$ ,  $>\text{CH}-$ ,  $-\text{C}=\text{C}-$  groups to dispersion interactions; the increments of  $-\text{CN}$ ,  $-\text{C}_6\text{H}_5$ ,  $-\text{Cl}$ ,  $-\text{COOCH}_3$  groups to polar interactions; the increments of  $-\text{OH}$ ,  $-\text{COOH}$  groups to hydrogen bonding interactions.

We tested the models for solubility parameters using a sample of the experimental data given in [14]. This sample contains the experimental data on the solubility parameters of the most common types of polymers from various sources. The authors give the minimum and maximum solubility parameters of the polymers. According to these data, we calculate the reproducibility dispersions of the experimental data. The solubility parameter estimates were calculated using the increments  $F_i$  (see Table 1) for polymers with the corresponding atomic groups in the link composition by formula (10). The value of the variance of the model validity (10) with the parameters from Table 1 for a sample of 25 polymers is 3.78 with an error variance of 3.77. The value of statistics is  $S_{ad}^2/S_{err}^2 = 1.001$ . The quantile value of the Fisher distribution with a significance level of 0.05 is 2.11, which indicates the adequacy of the mathematical model used, and consequently its applicability for calculating the solubility parameters of new polymers.

The following formulas were used to calculate the solubility parameters of butadiene nitrile copolymers containing different types of monomer links:

$$\delta_d = \frac{1}{V_m} \sum_{i,j} F_i^d n_i x_{ij}, \quad (11)$$

$$\delta_p = \frac{1}{V_m} \sum_{i,j} F_i^p n_i x_{ij}, \quad (12)$$

$$\delta_h = \frac{1}{V_m} \sum_{i,j} F_i^h n_i x_{ij}, \quad (13)$$

where  $\delta_d, \delta_p, \delta_h$  are the components of the vector solubility parameter, responsible for the contributions of dispersion, polar, and hydrogen bonding interactions;  $F_i^d, F_i^p, F_i^h$  are the increments of molecular attraction constants of the  $i$ -th atomic group, respectively, related to each



of the above groups of intermolecular interactions,  $x_{ij}$  is the relative proportion of the  $i$ -th atomic group in the  $j$ -th type copolymer link.

The total solubility parameter was calculated as the sum of the contributions of three (or in the special case two, if the copolymer has not units containing atomic groups capable to form the hydrogen bonds)

$$\delta = \delta_d + \delta_p + \delta_h. \quad (14)$$

Since different manufacturers of butadiene-nitrile copolymers use their own trade names of industrial rubber grades, the following symbols for copolymers have been adopted in the present work: BNR-20, BNR-30, BNR-40 for copolymers having respectively 20, 30 and 40 per cent of acrylic acid nitrile links in their composition; for hydrogenated copolymers in which the atomic groups of the double bond  $-\text{CH}=\text{CHN}-$  are replaced by atomic groups  $-\text{CH}_2-\text{CH}_2-$ , the first letter "H" was added to the copolymer name; the carboxylated copolymers containing acrylic acid units had symbols like "-5C" added to the end of the copolymer name, where the number indicates the percentage of acrylic acid units; hydroxylated copolymers had symbols like "-5H" added to the end of the copolymer name, where the number indicates the percentage of vinyl alcohol units in the copolymer (Table 3).

**Table 3.** Calculated solubility parameters for different types of butadiene nitrile copolymers

Copolymer type	$\delta$	$\delta_d$	$\delta_p$	$\delta_h$
BNR-20	19.00	16.33	2.67	0.00
BNR-30	19.67	15.59	4.08	0.00
BNR-40	20.38	14.82	5.55	0.00
HBNR-20	18.12	15.71	2.41	0.00
HBNR-30	18.82	15.10	3.73	0.00
HBNR-40	19.57	14.44	5.13	0.00
BNR-20-5C	19.65	15.95	2.61	1.10
BNR-30-5C	20.32	15.22	3.99	1.12
BNR-40-5C	21.02	14.46	5.42	1.14
BNR-20-5H	19.58	16.20	2.65	0.73
BNR-30-5H	20.26	15.47	4.05	0.74
BNR-40-5H	20.97	14.70	5.51	0.76

The free energy change during mixing was calculated within the framework of the Flory-Huggins lattice model [29].

$$\Delta G_M = \Delta H_M - T\Delta S_M = nRT \left[ \frac{\varphi}{N_p} \ln \varphi + (1 - \varphi) \ln(1 - \varphi) + \chi \varphi(1 - \varphi) \right], \quad (15)$$

$$\Delta H_M = nRT \chi \varphi(1 - \varphi), \quad (16)$$

$$T\Delta S_M = nRT \left[ \frac{\varphi}{N_p} \ln \varphi + (1 - \varphi) \ln(1 - \varphi) \right], \quad (17)$$



where  $n$  is the number of moles of the lattice;  $\varphi$  is the polymer volume fraction;  $N_p$  is the degree of polymerisation;  $\chi$  is the Flory-Huggins index of the polymer-solvent interaction.

The Flory-Huggins index was calculated through the solubility parameters of the polymer and  $\delta_1$  the solvent  $\delta_2$  using the formula

$$\chi = \frac{V_s}{RT} (\delta_1 - \delta_2)^2, \quad (18)$$

where  $V_s$  is the molar volume of the solvent.

Dibutyl phthalate, which is used as a plasticizer for butadiene nitrile rubbers, and isooctane were regarded as "good" and "bad" solvents in the thermodynamic sense, respectively. In the first case for all types of butadiene nitrile rubbers under study the change of free energy at mixing is negative within the whole range of solvent concentration, which indicates complete compatibility of all rubbers with plasticizer (Fig. 1 shows the dependencies for rubbers containing 30% of acrylic acid nitrile units). In the second case (Fig. 2) there is a phase separation and the area of partial solubility is only a small fraction of the concentration range. For both solvents, the best compatibility occurs for hydrogenated BNRs. Indeed, although the hydrogenation process improves the useful properties of butadiene nitrile rubbers (primarily their heat resistance), their resistance to non-polar solvents will be reduced.

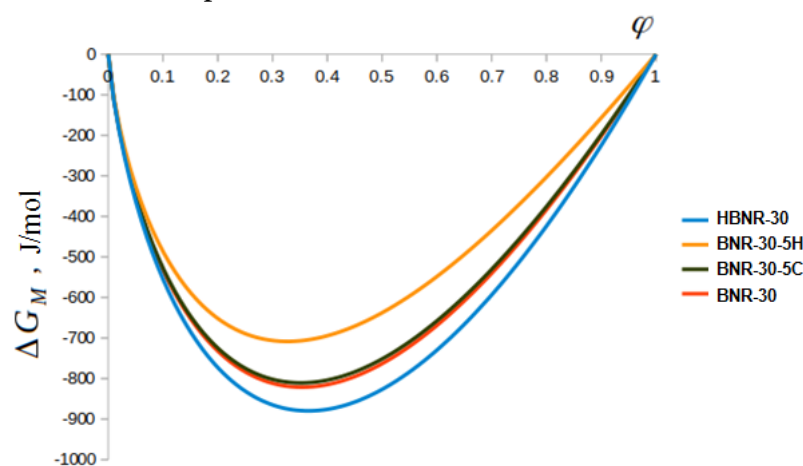


Fig. 1. The dependence of change in free mixing energy of butadiene nitrile rubbers with dibutyl phthalate on the solvent volume fraction,  $n = 1$ ,  $N_p = 1000$

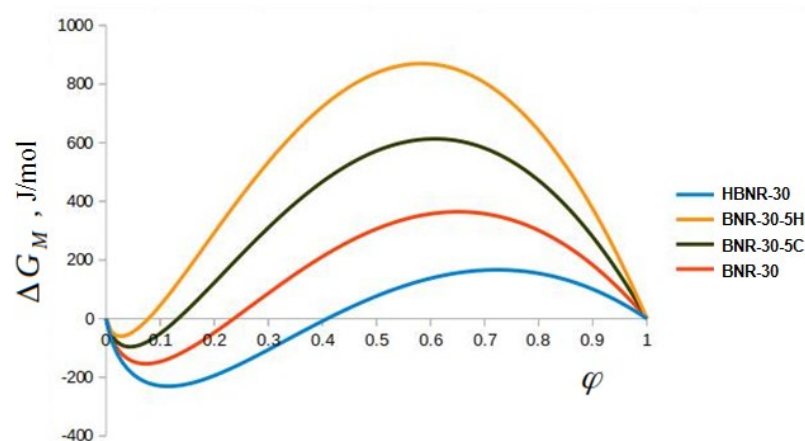


Fig. 2. The dependence of change in free mixing energy of butadiene nitrile rubbers with isooctane on the solvent volume fraction,  $n = 1$ ,  $N_p = 1000$



According to the study, hydroxylated butadiene nitrile rubbers with 30% acrylonitrile units are the most resistant to non-polar solvents. They are followed by carboxylated rubbers, and rubbers containing no carboxyl or hydroxyl groups occupy an intermediate position between BNR-30-5C and HBNR-30.

### Conclusions

Calculation of atomic group increments by the group additivity method on the samples containing only compounds with types of functional groups corresponds to the target compounds and increases the accuracy of prediction their physico-chemical properties. It was demonstrated on the example of enthalpy of evaporation, molar volume, and solubility parameters of butadiene nitrile rubbers with functional groups.

When solubility parameters are calculated by increments of the Small molecular attraction constants, the relative error of the predicted values is smaller compared to calculating these parameters from the cohesion energy density through the enthalpy of evaporation and the molar volume.

According to the study, the butadiene nitrile rubbers with hydroxyl groups have the greatest resistance to non-polar solvents compared with other types of modified butadiene nitrile rubbers. Hydrogenated butadiene nitrile rubbers are less resistant to non-polar solvents than conventional rubbers.

### References

1. **Kligender, R.C.** (2019) *Handbook of Specialty Elastomers*. Boca Raton: CRC Press.
2. **Koshelev, F.F., Kornev, A.E. & Bukanov, A.M.** (1978) *General technology of rubber*. 4-th ed., rev. and supplement. M.: Khimiya (in Russian).
3. **Mandal, U.K.** (2000) Ionic elastomer based on carboxylated nitrile rubber: infrared spectral analysis, *Polymer International*, 49(12), pp. 1653–1657. DOI: doi.org/10.1002/1097-0126(200012)49:12<1653::AID-PI586>3.0.CO;2-U.
4. **Prochon, M., Przepiorkowska, A. & Zaborski, M.** (2007) Keratin as a filler for carboxylated acrylonitrile-butadiene rubber XNBR, *Journal of Applied Polymer Science*, 106(6), pp. 3674–3687. DOI: 10.1002/app.26324.
5. **Wang, J., Jia, H. Tang, Y., Ji, D., Sun, Y., Gong, X. & Ding, L.** (2013) Enhancements of the mechanical properties and thermal conductivity of carboxylated acrylonitrile butadiene rubber with the addition of graphene oxide, *Journal of Material Science*, 48, pp. 1571–1577. DOI: 10.1007/s10853-012-6913-1.
6. **Laskowska, A., Zaborski, M., Boiteux, G., Gain, O., Marzec, A. & Maniukiewicz, W.** (2014) Ionic elastomers based on carboxylated nitrile rubber (XNBR) and magnesium aluminum layered double hydroxide (hydrotalcite), *eXPRESS Polymer Letters*, 8, pp. 374–386. DOI: 10.3144/expresspolymlett.2014.42.
7. **Gaca, M. & Zaborski, M.** (2016) The properties of elastomers obtained with the use of carboxylated acrylonitrile-butadiene rubber and new crosslinking substances, *Polimery*, 61(1), pp. 31-38. DOI: 10.14314/polimery.2016.031.
8. **Tripathi, G. & Srivastava, D.** (2011) Study on the Effect of Carboxyl Terminated Butadiene Acrylonitrile (CTBN) Copolymer Concentration on the Decomposition Kinetics Parameters of Blends of Glycidyl Epoxy and Non-Glycidyl Epoxy Resin, *International Journal of Organic Chemistry*, 1, pp. 105-112. DOI: 10.4236/ijoc.2011.13016.
9. **Brzić, S.J., Jelisavac, L.N., Galović, J.R., Simić, D.M. & Petković, J.L.** (2014) Viscoelastic properties of hydroxyl-terminated poly(butadiene)-based composite rocket propellants, *Chemical Industry*, 68(4), pp. 435-443. DOI: 10.2298/HEMIND130426067B.
10. **Brzić, S., Ušćumlić, G., Milojković, A., Rodić, V. & Bogosavljević, M.** (2015) Viscoelastic Properties of Carboxyl-Terminated (Butadiene-co-Acrylonitrile)-Based Composite Rocket Propellant Containing





- Tris(2,3-Epoxypropyl) Isocyanurate as Bonding Agen, *Scientific Technical Review*, 65(4), pp. 28-36. DOI: 10.5937/STR1504028B.
11. **Brzić, S.J., Uščumlić, G.S., Dimić, M.V., Tomić, M., Rodić, V.Ž. & Fidanovski, B.Z.** (2016) Viscoelastic behaviour of carboxyl-terminated (butadiene-co-acrylonitrile)-based composite propellant binder containing polyglycidyl-type bonding agent, *Chemical Industry*, 70(5), pp. 547–556. DOI: 10.2298/HEMIND150918062B.
  12. **Ai, C., Li, J., Gong, G., Zhao, X. & Liu, P.** (2018) Preparation of hydrogenated nitrile-butadiene rubber (H-NBR) with controllable molecular weight with heterogeneous catalytic hydrogenation after degradation via olefin cross metathesis, *Reactive and Functional Polymers*, 129, pp. 53-57. DOI: doi.org/10.1016/j.reactfunct-polym.2017.12.016.
  13. **Yun, J., Zolfaghari, A. & Sane, S.** (2022) Study of hydrogen sulfide effect on acrylonitrile butadiene rubber/hydrogenated acrylonitrile butadiene rubber for sealing application in oil and gas industry, *Journal of Applied Polymer Science*, 139(30), e52695. DOI: doi.org/10.1002/app.52695.
  14. **Van Krevelen, D.W. & Nijenhuis, K.Te.** (2009) *Properties of polymers. Their correlation with chemical structure; their numerical estimation and prediction from additive group contributions*. Amsterdam: Elsevier.
  15. **Baskin, I.I., Majidov, T.I. & Varnek, A.A.** (2015) *Introduction to Chemoinformatics. Part 3. Structure-property modeling*. Kazan: Izdatel'stvo Kazanskogo universiteta (in Russian).
  16. **Solovyev, M.E. & Dmitriev, K.E.** (2021) *Computer modelling in chemistry*. Yaroslavl: Izdat. dom YaGTU (in Russian).
  17. **Batov, D.V.** (2021) Analysis, systematization and prediction of thermodynamic characteristics of organic compounds and their solutions based on additive-group method, *From Chemistry Towards Technology Step-By-Step*, 2(2), pp. 8-59 [online]. Available at: <http://chemintech.ru/index.php/tor/2021-2-2> DOI: 10.52957/27821900\_2021\_02\_8 (in Russian).
  18. **Ilyin, A.A. Sizov, E.A. Soloviev, M.E. & Mogilevich, M.M.** (2000) Increments of enthalpies of organic compounds evaporation. *Zhurnal obschey khimii*, 70(7), pp. 1088-1091 (in Russian).
  19. **Korolev, G.V., Ilyin, A.A., Mogilevich, M.M., Chebunin, R.V. & Solovyev, M.E.** (2003) Peculiarities of intermolecular interactions in organic compounds with anomalously low boiling points, *Zhurnal obschey khimii*, 73(3), pp. 360-366 (in Russian).
  20. **Ilyin, A.A., Solovyev, M.E., Mogilevich, M.M., Semeykin, I.N. & Korolev, G.V.** (2002) Modelling of associative structures of fluoroalkyl methacrylates, *Visokomolekulyarnie soedineniya. Ser. B*, 44(4), pp. 693-696 (in Russian).
  21. **Lebedev, Y.A. & Miroshnichenko, E.A.** (1981) *Thermochemistry of vaporization of organic substances, heat of evaporation, sublimation and pressure of saturated steam*. M.: Nauka (in Russian).
  22. **Mackay, D., Shiu, W.Y., Ma, K.-C. & Lee, S. C.** (2006) *Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals. Second Ed. Volumes I, III, IV*. Boca Raton: CRC Press.
  23. *NIST Chemistry WebBook. NIST Standard Reference Database Number 69* [online]. Available at: <https://webbook.nist.gov/chemistry/> Last update to data: 2022 (accessed 10.10.2022). DOI: <https://doi.org/10.18434/T4D303>.
  24. **Solovyev, M.E.** (2012) *Experimental and statistical methods in chemical engineering research using Open Source software*. Yaroslavl: Izdatel'stvo YaGTU [online]. Available at: <https://www.elibrary.ru/item.asp?id=45667592> (accessed 10.10.2022) (in Russian).
  25. **Small, P.A.** (1953) Some factors affecting the solubility of polymers, *Journal of Applied Chemistry*, 3(2), pp. 71-80. doi.org/10.1002/jctb.5010030205.
  26. **Fedors, R.F.** (1974) A method for estimating both the solubility parameters and molar volumes of liquids, *Polymer Engineering and Science*, 14(2), pp. 147-154. DOI: doi.org/10.1002/pen.760140211.
  27. **Dmitriev, K.E. & Soloviev, M.E.** (2022) Prediction of thermodynamic properties of fatty acids and their esters by additive-group contribution method, *Matematika i estestvenniye nauki: teoriya i praktika: mezhvuzovskiy sbornik nauchnih trudov. Vol. 17*. Yaroslavl: Izdat. dom YaGTU, pp. 136-142 (in Russian).
  28. **Solov'ev, M.E., Rauhvarger, A.B. & Irzhak, V.I.** (2021) Simulation of local dynamics of intermolecular interactions in nitrile-butadiene copolymers with carboxyl and hydroxyl groups, *Polymer Science. Series A*, 63(4), pp. 435-443. DOI: 10.1134/S0965545X21040076.
  29. **Flory, P.J.** (1953) *Principles of Polymer Chemistry*. NY, Ithaca: Cornell University Press.

Received 21.11.2022

Approved 25.11.2022

Accepted 09.12.2022