



User Manual: Calculation №106
**«Determination of LPG Composition, Calculation of Density,
Pressure, and Octane Number»**

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1. Introduction

The “Determination of LPG Composition, Calculation of Density, Pressure, and Octane Number” program is designed to analyze chromatograms obtained using Chromos SW to determine the composition of liquefied petroleum gases (LPG) and the concentration of components in accordance with GOST R 54484-2011, GOST 33012-2014, GOST 10679-76, or GOST 10679-2019. Basing on the concentrations and the composition obtained, the LPG pressure and density are calculated in accordance with GOST 28656-2019, and the octane number is calculated in accordance with GOST EN 589-2014 or GOST R 52087-2018.

Before getting started, it is recommended to study the foregoing documents.

This software works as an extension and can only be launched on a registered copy of Chromos SW. To run the program you need a key.

The plug-in installation file and documentation are available on the Internet at: kb.has.ru/soft:dop_raschjot_106.

E-mail your suggestions and comments on the software to: soft@has.ru

2. Installing the Software

You need 5 Mb of free space on your local drive. To install the software, do the following:

1. Run the installation file.
2. Choose your language.
3. In the installer (Fig. 1), specify the components to be installed and click **Install**.

Note: When choosing the *Clean install* option, all user data (settings, aliases, coefficients) specified in the previous version of the program are set to default values.

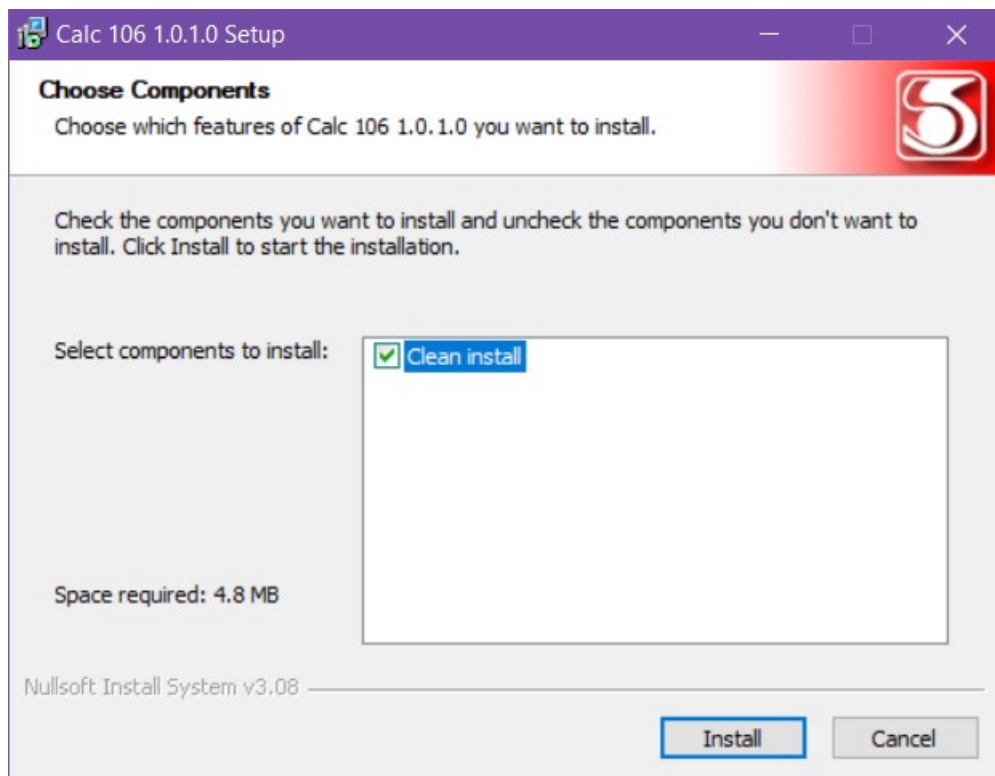


Fig. 1: Installation

4. When installed, click **Finish**.

After the software is successfully installed you can run it from Chromos SW.

3. Running the Plug-in

3. Running the Plug-in

This software works as an extension for Chromos SW. To run the extension, do the following:

1. Connect the key to a USB port.
2. Run Chromos SW.
3. In the *Data* menu, navigate to **Calculations > LPG composition** (Fig. 2). The main program window opens (Fig. 3).

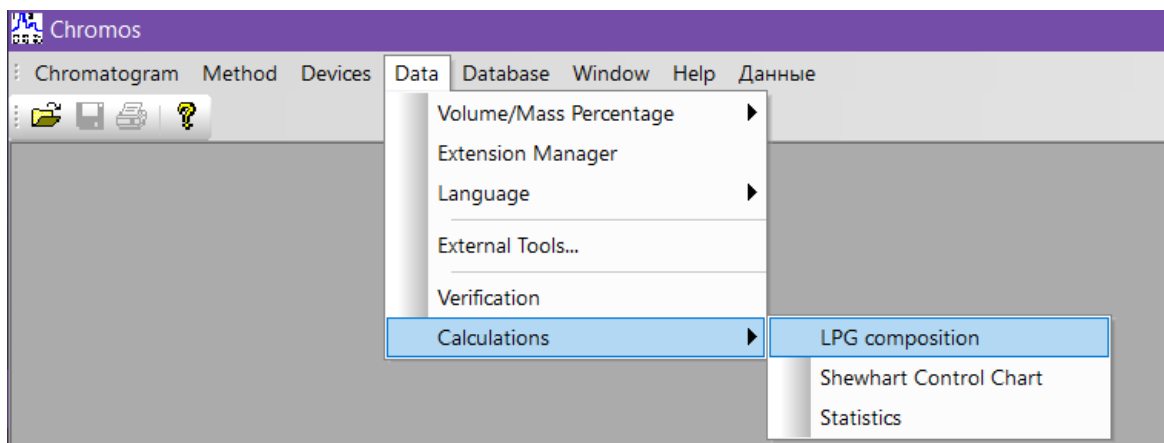


Fig. 2. Running the plug-in from Chromos SW

4. Program Overview

The main program window (Fig. 3) contains the following elements:

1. Chromatograms/Mixtures tabs;
2. Chromatogram controls;
3. Refresh button;
4. Program settings;
5. Report controls;
6. List of opened chromatograms/mixtures;
7. Operation tabs.

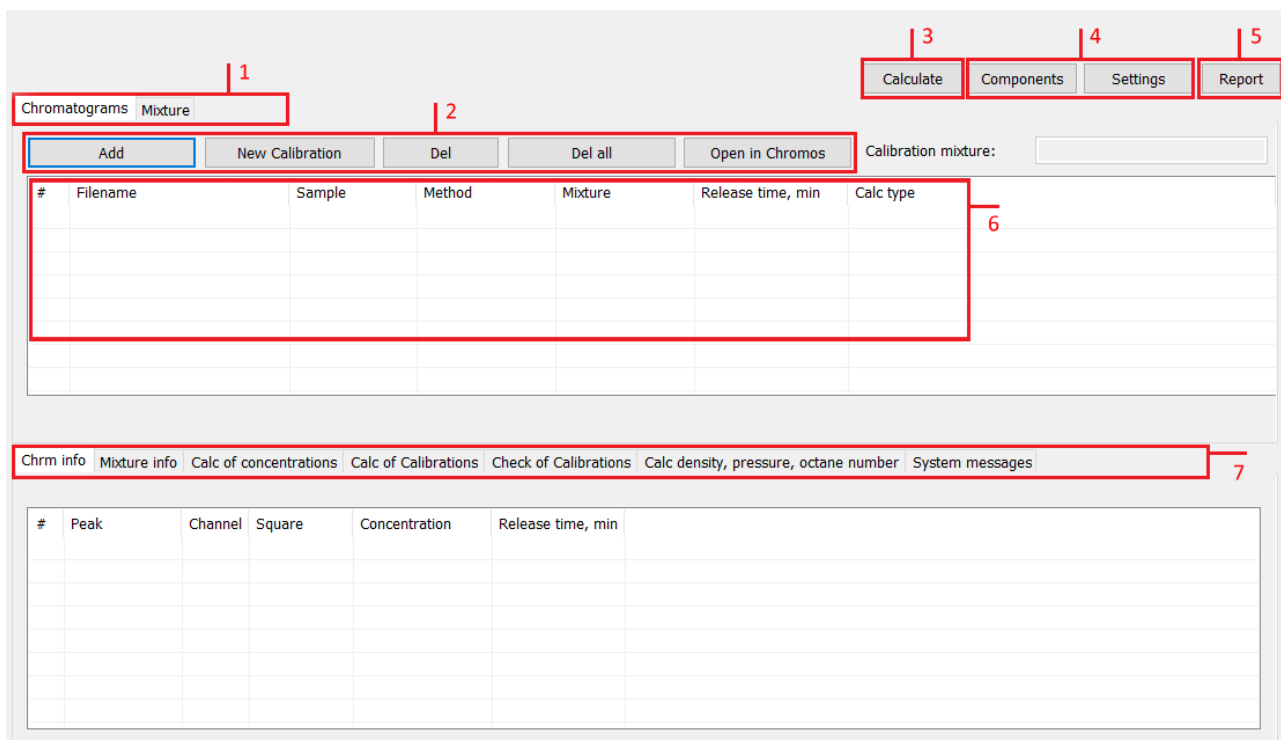


Fig. 3. Main program window

The main program window contains the following operation tabs:

- *Chrm info* — the tab displays chromatogram information:
 - # — string number;
 - *Peak* — sample component name;
 - *Channel* — chromatogram channel;
 - *Square* — peak area;
 - *Concentration* — component concentration;
 - *Release time, min* — peak exit time (in minutes);
- *Mixture info* — the tab displays mixture information:
 - # — string number;
 - *Component* — component name;
 - *Concentration, mol%* — molar fraction of a component;
 - *Uncertainty, %rel.* — uncertainty;

4. Program Overview

- *Calc of Concentrations* — calculated values of concentrations (depending on the calculation method selected):
 - *Component* — sample component name;
 - *Avrg conc, mass.%* — average mass fraction of a component;
 - *Avrg conc, mol.%* — average molar fraction of a component;
 - *Divergence, mass.%* — divergence of successive measurements;
 - *Fact. repeat, %* — repeatability factor;
 - *Repeat limit, %* — repeatability limit (convergence);
 - *Rel. error, mass.%* — relative error;
 - *Conc, mass.%* — mass fraction of a component;
 - *Conc, mol.%* — molar fraction of a component;
 - *Conc, vol.%* — volume fraction of a component;
 - *Abs. exp. uncert, mass.%* — absolute expanded uncertainty of the measurement result of the mass fraction of the hydrocarbon component in LPG;
 - *Resp.* — compliance to the standard;
- *Calc of Calibrations:*
 - *Component* — sample component name;
 - *Grad. conc, mol.%* — calibration concentration (molar fraction);
 - *K avrg.* — average calibration factor;
- *Check of Calibrations:*
 - *Component* — sample component name;
 - *K old.* — initial calibration factor;
 - *K new.* — normalized calibration factor;
 - *Rel. range (R new)* — relative range;
 - *Tolerance (R* new)* — relative range tolerance;
 - *Resp.* — compliance to the standard;
- *Calc density, pressure, octane number* — console for calculating the density and pressure of saturated vapors depending on temperature, as well as the results of calculating concentrations:
 - *#* — string number;
 - *Component* — sample component name;
 - *Conc. mol.%* — molar fraction of a component;
 - *Conc, mass.%* — mass fraction of a component;
- *System messages* — the tab displays errors and warning messages about any inconsistency or the impossibility of performing calculations due to missing data.

5. Measurement Procedure

To carry out measurements, two types of chromatograms are used: calibration and calculation (analysis). Depending on the method, to carry out the analysis, you need to add one calibration chromatogram and one calculation chromatogram. To comply with GOST R 54484-2011 clause 9.5.3, you should add at least three calibration chromatograms.

Using the *New calibration* button, you can add chromatograms to check calibrations (see GOST R 54484-2011).

Detailed information about added chromatograms and mixtures is displayed on the *Chromatograms* and *Mixtures* tabs, respectively.

On the *Calc of density, pressure, octane number* tab in the main program window, you can set temperatures for calculating density, as well as normal and excess saturated vapor pressure. To set temperatures, click **Set Temperatures**, enter temperatures in the pop-up window, and click **OK**.

Also on the *Calc of density, pressure, octane number* tab, the octane number calculated by the motor method (MON) and molecular weight are displayed.

You can select the calculation method in the *Configuring the Analysis Settings* section (8.2). If you change the calculation parameters, in the main program window, click **Calculate** to update the results.

You can configure component names and sensitivity coefficients in the *Managing the Components* section (8.1). If there is a dash in the sensitivity coefficient field of a component, it means that the value was not specified in the selected GOST. Such components are skipped in the calculations. If a component must be taken into account, you need to specify its sensitivity factor.

Note: The program converts mass fractions into mole and volume fractions according to the following formulas (Fig. 4):

Expression	Molar fraction $x, \frac{kg-mol}{kg-mol\ of\ mixture}$	Mass fraction $\omega, \frac{kg}{kg\ of\ mixture}$	Volume fraction $\varphi, \frac{m^3}{m^3\ of\ mixture}$
Molar fraction $x, \frac{kg-mol}{kg-mol\ of\ mixture}$	–	$\frac{\omega_i}{M_i}$ $\sum_{i=1}^{i=k} \frac{\omega_i}{M_i}$	$\frac{\varphi_i \rho_i}{M_i}$ $\sum_{i=1}^{i=k} \frac{\varphi_i \rho_i}{M_i}$
Mass fraction $\omega, \frac{kg}{kg\ of\ mixture}$	$\frac{x_i M_i}{\sum_{i=1}^{i=k} C_i M_i}$	–	$\frac{\varphi_i \rho_i}{\sum_{i=1}^{i=k} \varphi_i \rho_i}$
Volume fraction $\varphi, \frac{m^3}{m^3\ of\ mixture}$	$\frac{x_i M_i}{\rho_i}$ $\sum_{i=1}^{i=k} \frac{x_i M_i}{\rho_i}$	$\frac{\omega_i}{\rho_i}$ $\sum_{i=1}^{i=k} \frac{\omega_i}{\rho_i}$	–

Fig. 4: Fraction converting formulas

6. Adding Data

6. Adding Data

To carry out the calculation, you need to add chromatograms. To add data, do the following:

1. Click **Add**. The *Select Analysis* window opens (Fig. 5).
2. (Optional) To add a chromatogram for calibration check in accordance with GOST R 54484-2011, click **New Calibration**. The *Select Analysis* window opens (Fig. 5).
3. In the *Select Analysis* window, select the chromatograms and click **OK**. The added files are displayed in the list of chromatograms in the main program window.

To select chromatograms, you can use filters by method, date, type, sampling place and sampling point, operator and sample. You can also select multiple files at once using combinations Ctrl + Mouse and Shift + ←↑↓→

4. To delete the chromatogram, select it and click **Delete**.
5. To clear the list of chromatograms, click **Delete All**.
6. To open the chromatogram in Chromos SW, double-click it or select it and click **Open in Chromos**.

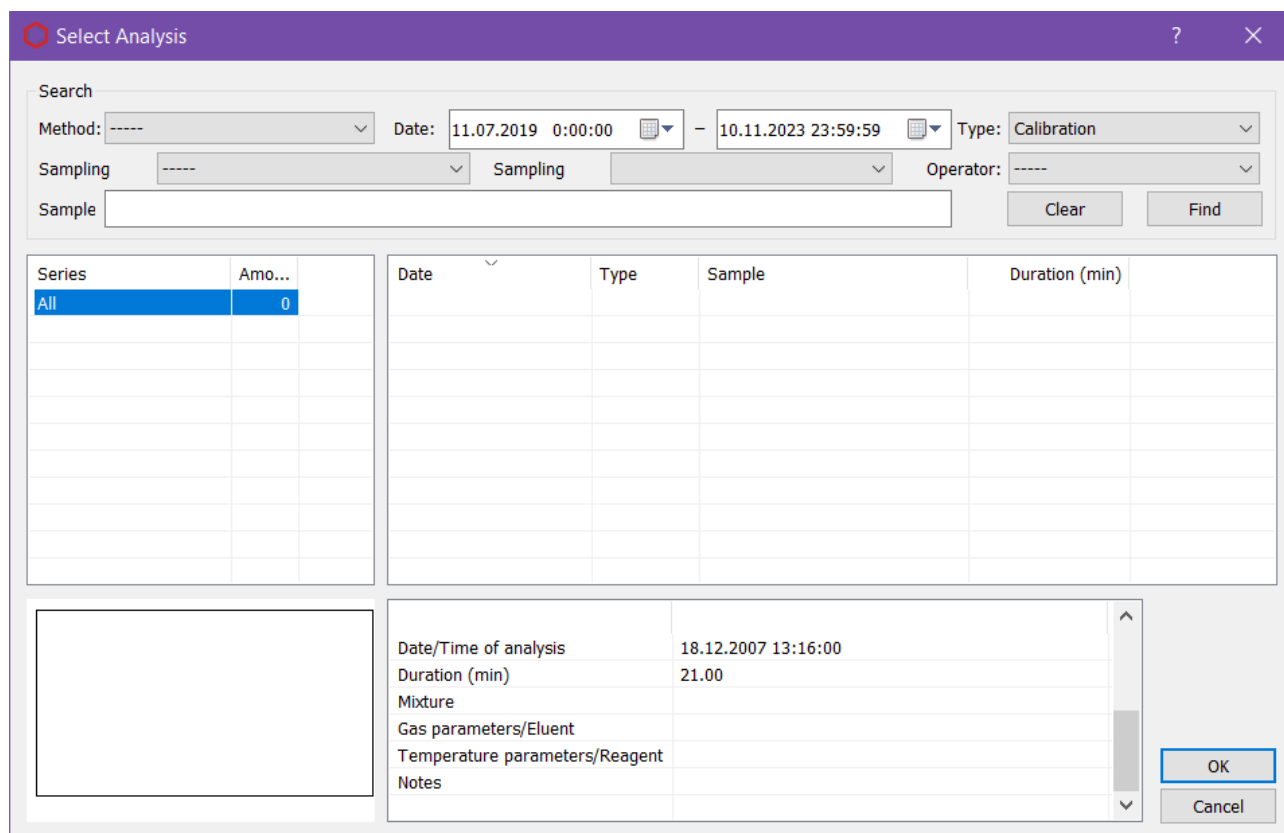


Fig. 5. Select Analysis

7. Reporting

You can write the calculated data to a report.

1. To generate the report, click **Report**. The *Report Settings* window opens (Fig. 6).

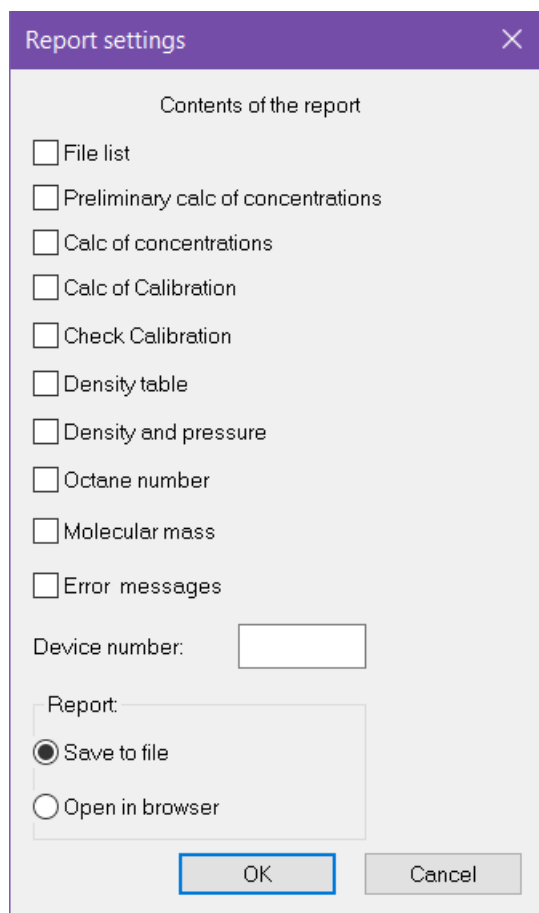


Fig. 6: Report settings

2. In the *Report Settings* window, select the data to add to the report.
3. In the *Device Number* field, enter the device number.
4. Choose the action:
 - To open the report in a web browser, select **Open in browser** and click **OK**.
 - To save the report, select **Save to file** and click **OK**.

By default the report is named like **Report106_17102023_114811.html**, with:

- *Report106* – program name;
- *17102023* — date in DDMMYYYY format;
- *114811* — time in HHMMSS format;
- *html* – file extension.

8. Configuring the Program Settings

Setting up the program includes managing the components and configuring the calculation parameters.

8.1. Managing the Components

The component list contains predefined component entries. To manage the components, do the following:

1. In the main program window, click **Analysis Settings**. The *Analysis Settings* window opens (Fig. 7).
2. To edit component parameters, double-click the corresponding field.

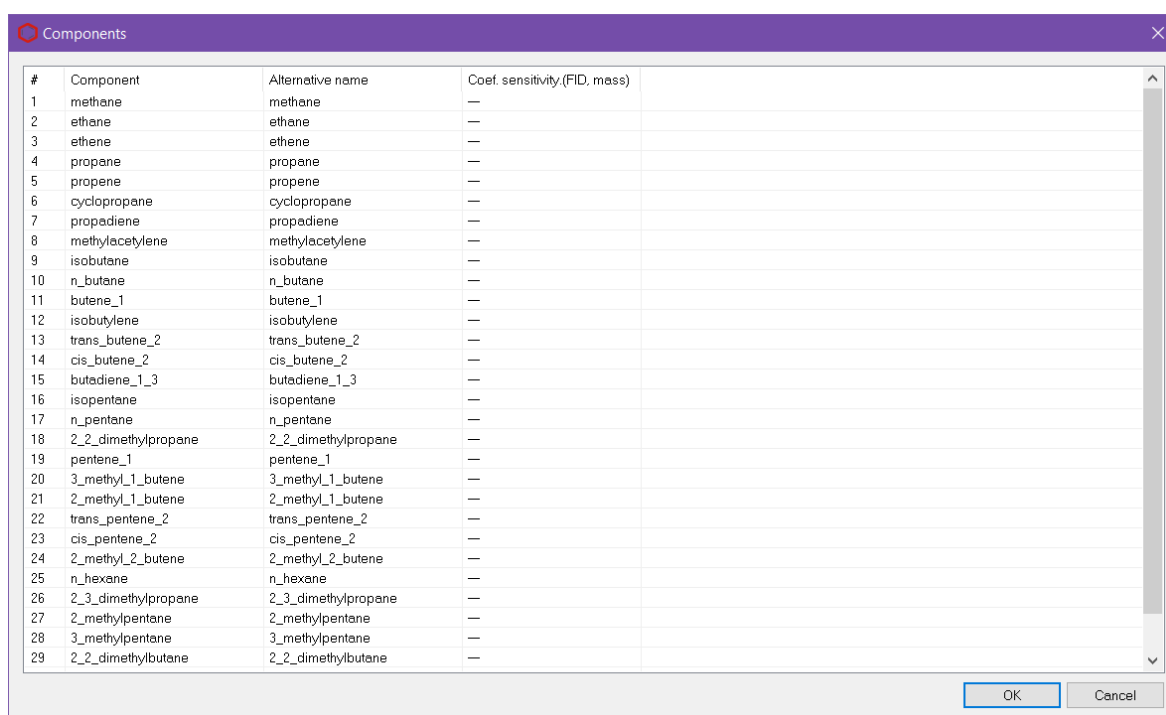
- In the *Alternative Name* field, enter the component name.

Components should have unique names.

- In the *Coef. Sensitivity (TCD/FID mass)* field, enter the detector sensitivity coefficient.

You are able to configure this parameter if you select either the *GOST 10679-76* or the *GOST 10679-2019 (relative grad.)* calculation method.

3. To save the changes, click **OK**.



#	Component	Alternative name	Coef. sensitivity.(FID, mass)
1	methane	methane	—
2	ethane	ethane	—
3	ethene	ethene	—
4	propane	propane	—
5	propene	propene	—
6	cyclopropane	cyclopropane	—
7	propadiene	propadiene	—
8	methylacetylene	methylacetylene	—
9	isobutane	isobutane	—
10	n_butane	n_butane	—
11	butene_1	butene_1	—
12	isobutylene	isobutylene	—
13	trans_butene_2	trans_butene_2	—
14	cis_butene_2	cis_butene_2	—
15	butadiene_1_3	butadiene_1_3	—
16	isopentane	isopentane	—
17	n_pentane	n_pentane	—
18	2_2_dimethylpropane	2_2_dimethylpropane	—
19	pentene_1	pentene_1	—
20	3_methyl_1_butene	3_methyl_1_butene	—
21	2_methyl_1_butene	2_methyl_1_butene	—
22	trans_pentene_2	trans_pentene_2	—
23	cis_pentene_2	cis_pentene_2	—
24	2_methyl_2_butene	2_methyl_2_butene	—
25	n_hexane	n_hexane	—
26	2_3_dimethylpropane	2_3_dimethylpropane	—
27	2_methylpentane	2_methylpentane	—
28	3_methylpentane	3_methylpentane	—
29	2_2_dimethylbutane	2_2_dimethylbutane	—

Fig. 7: Components

8.2. Configuring the Analysis Settings

You can configure the analysis settings and select the calculation method.

1. In the main program window, click **Settings**. The *Calc Settings* window opens (Fig. 8).
2. In the *Calc Settings* window, in the *Calc method* section, select the calculation method:
 - GOST R 54484-2011 Relative coefficients;
 - GOST R 54484-2011 Calibration coefficients;
 - GOST 33012-2014 Method A (packed column);
 - GOST 33012-2014 Method B (capillary column);
 - GOST 10679-76;
 - GOST 10679-2019 (relative grad.) — relative calibration;
 - GOST 10679-2019 (absolute grad.) — absolute calibration.
3. For the *GOST R 54484-2011 Relative coeff.* method select the substance standard from the list.
4. For the *GOST 10679-76* and the *GOST 10679-2019 (relative grad.)* methods, select the type of detector:
 - Thermal conductivity detector (TCD);
 - Flame ionization detector (FID).
5. For the *GOST 10679-2019 (relative grad.)* calculation method, select the dimension of calibration concentrations:
 - Mass %;
 - Mol %.
6. In the *Octane number calc method* section, select the octane number calculation standard:
 - GOST EN 589 -2014;
 - GOST R 52087-2018.
7. In the *Rounding values* section, configure the rounding parameters:
 - In the *Round to sign* field, enter the number of decimal places;
 - To apply rounding in accordance with GOST 10679-2019, check the **Round by GOST 10679-2019** box;
 - To round the physical and chemical parameters in accordance with GOST 10679-2019, check the **Round phys and chem parameters by GOST 10679-2019** box.
8. To save the changes, click **OK**.

8.2. Configuring the Analysis Settings

Calc settings

Calc method:

GOST P 54484-2011 Relative coeff.
Substance standard:

GOST P 54484-2011 Calibration coeff.

GOST 33012-2014 Method A (packed col)

GOST 33012-2014 Method B (capillary col)

GOST 10679-76

GOST 10679-2019 (relative grad.)

GOST 10679-2019 (absolute grad.)

Detector type: TCD FID

Dimension of grad conc: mass % mol %

Octane number calc method:

GOST EN 589-2014

GOST P 52087-2018

Rounding values:

Round to sign:

Round by GOST 10679-2019

Round phys and chem parameters by GOST 10679-2019

OK Cancel

Fig. 8: Calculation settings

9. Program Identification

To view the program details, in the top left corner click on the icon, then in the context menu select **About 106**. The *About...* window opens (Fig. 9).

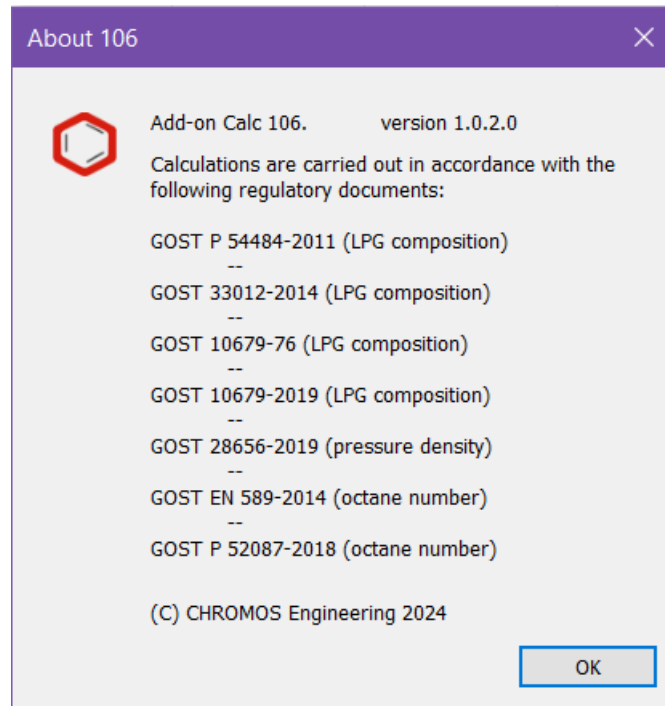


Fig. 9. About...