Getting started with Simulis® Thermodynamics

Use Case 9: Create a compound that is not available in databases

Software & Services In Process Simulation

We guide You to efficiency

ProSim

Introduction

This document presents the different steps to follow to create a new compound that is not present in databases and to determine its properties.

The steps are the following:

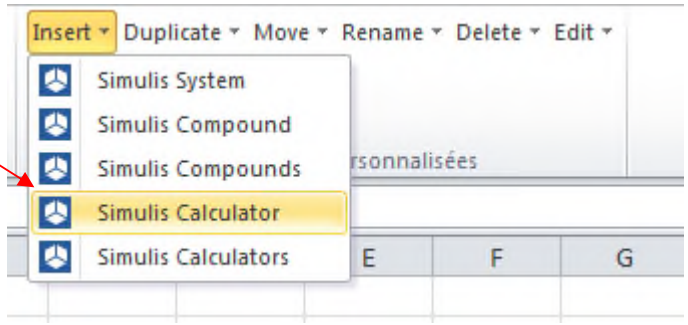
- Step 1: Add a new compound
- Step 2: Enter the SMILES of the compound
- Step 3: Determine constant properties
- Step 4: Decomposition into functional sub-groups
- Step 5: Temperature dependent properties

Step 1: Add a new compound

ACCESS THE THERMODYNAMIC CALCULATOR EDITOR:

- **<u>If you are using Simulis Thermodynamics in Excel</u>:**

Create the calculator object in a spreadsheet



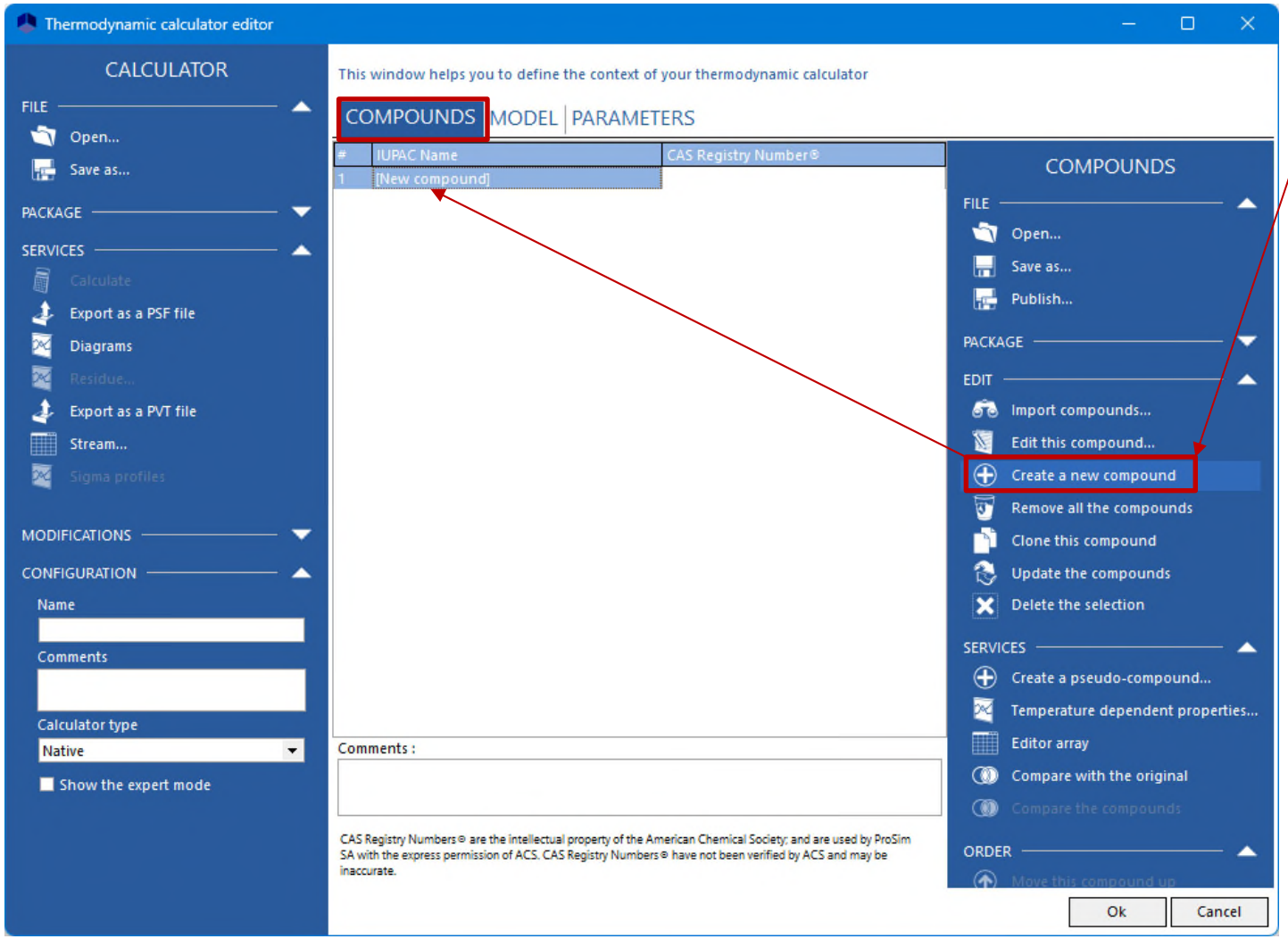
- **<u>If you are using Simulis Thermodynamics within another ProSim environment</u> (ProSimPlus, BatchReactor, BatchColumn etc…):**

Click on the thermodynamic icon to open the calculator editor:

or

Simulis Thermodynamics is a « software component » that you can integrate into different applications: ProSim software, Excel, Matlab, your own software, etc…

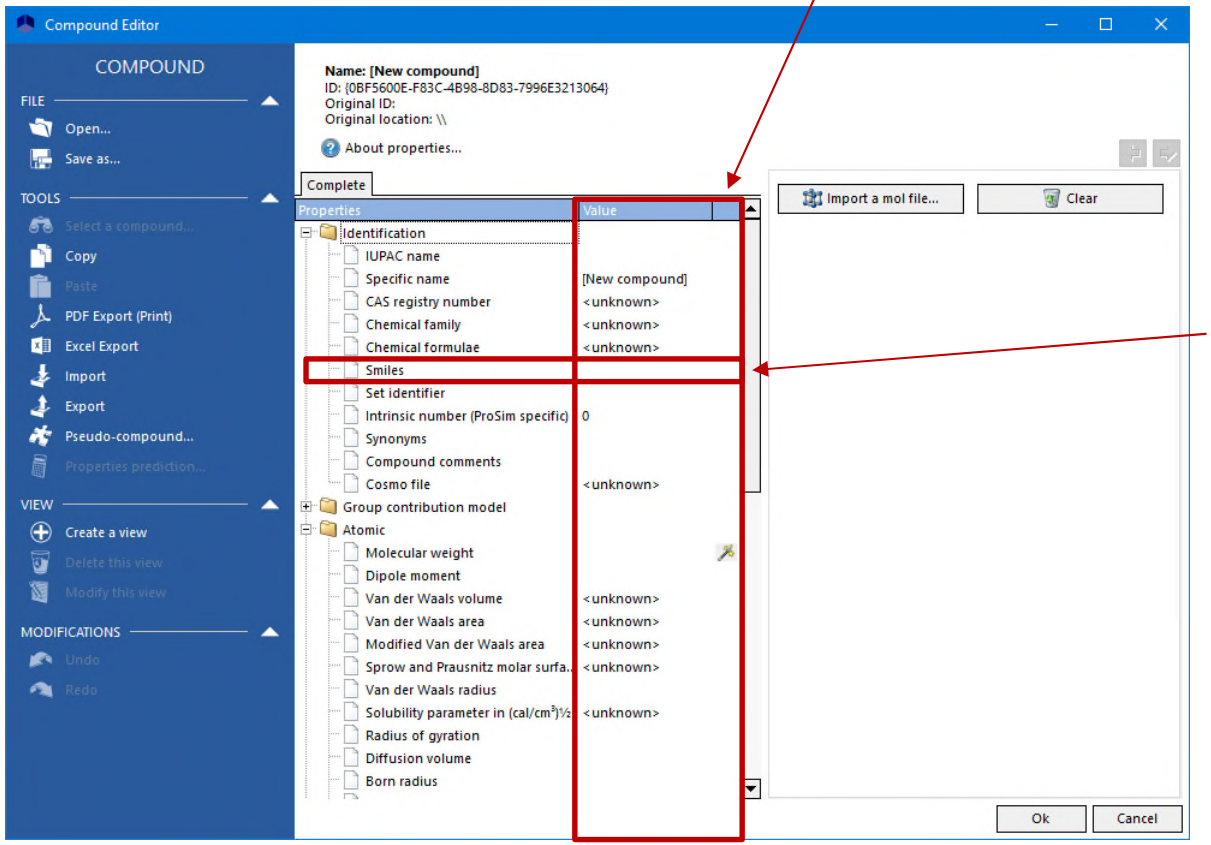
Step 1: Add a new compound



Create a new compound and edit this compound *(Double-click or right-click on the [New compound] added)*

Step 1: Add a new compound

1. Enter known information and properties of the new compound:
- *Name*
- *CAS Registry number*
- *Chemical formula*
- *Etc.*



2. Enter the SMILES of the compound
Allows estimation of complementary properties from group contribution methods

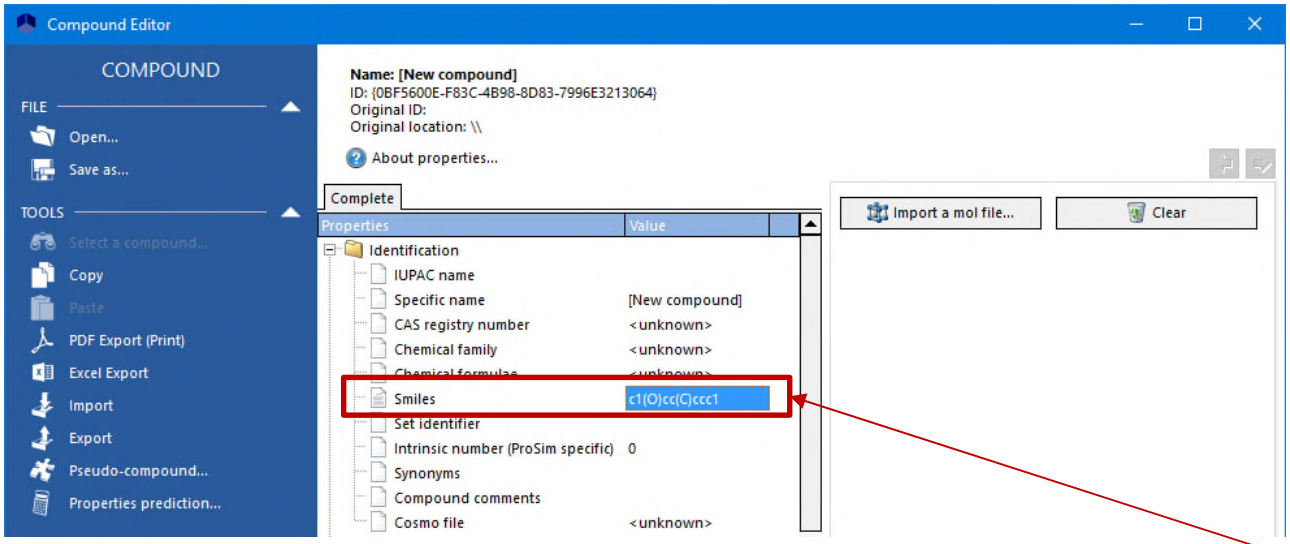
Step 2: Enter the SMILES of the compound

SMILES: Simplified Molecular Input Line Entry Specification

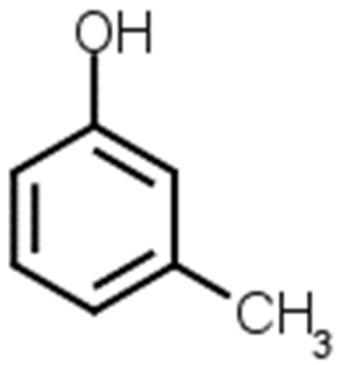
Weininger, J. Chem. Inf. Comput. Sci., 28 (1988)

Specification in form of a line notation for describing the structure of chemical species using short ASCII strings

https://en.wikipedia.org/wiki/Simplified_molecular-input_line-entry_system

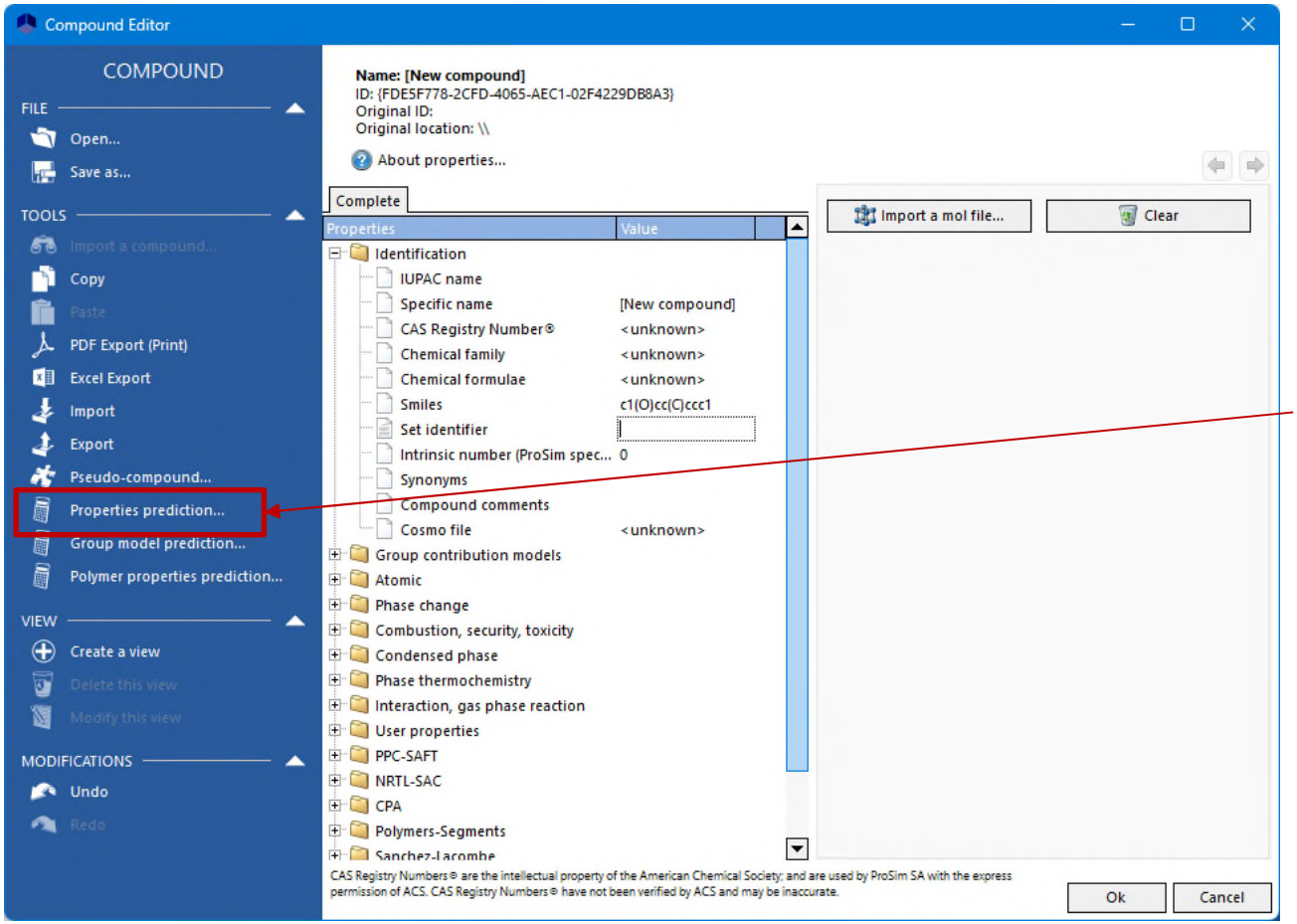


Example:



c1(O)cc(C)ccc1

Step 3: Determine constant properties



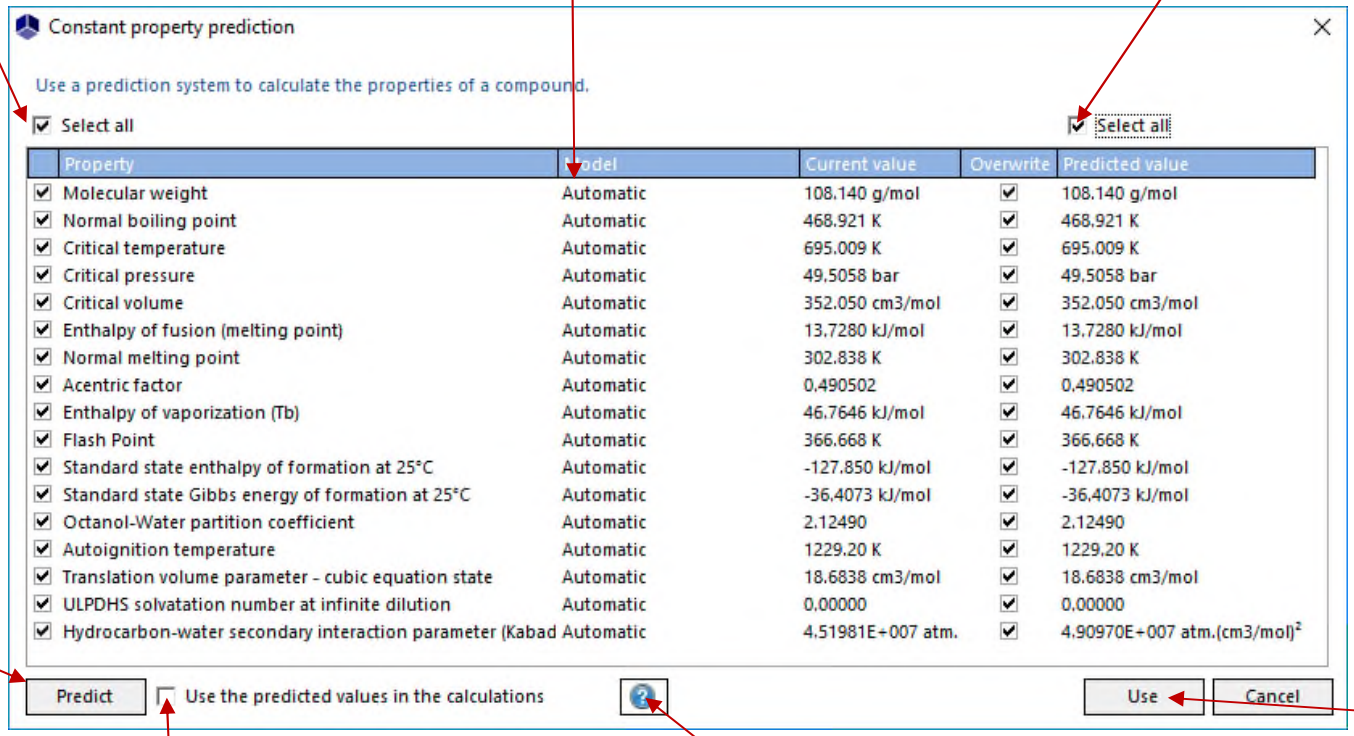
Click on
“Properties prediction…”

Step 3: Determine constant properties

1. Select all
(or only properties to be estimated)

2. Select predictive models
or keep automatic selection

5. Select all
(or only properties to be used)



4. Predict

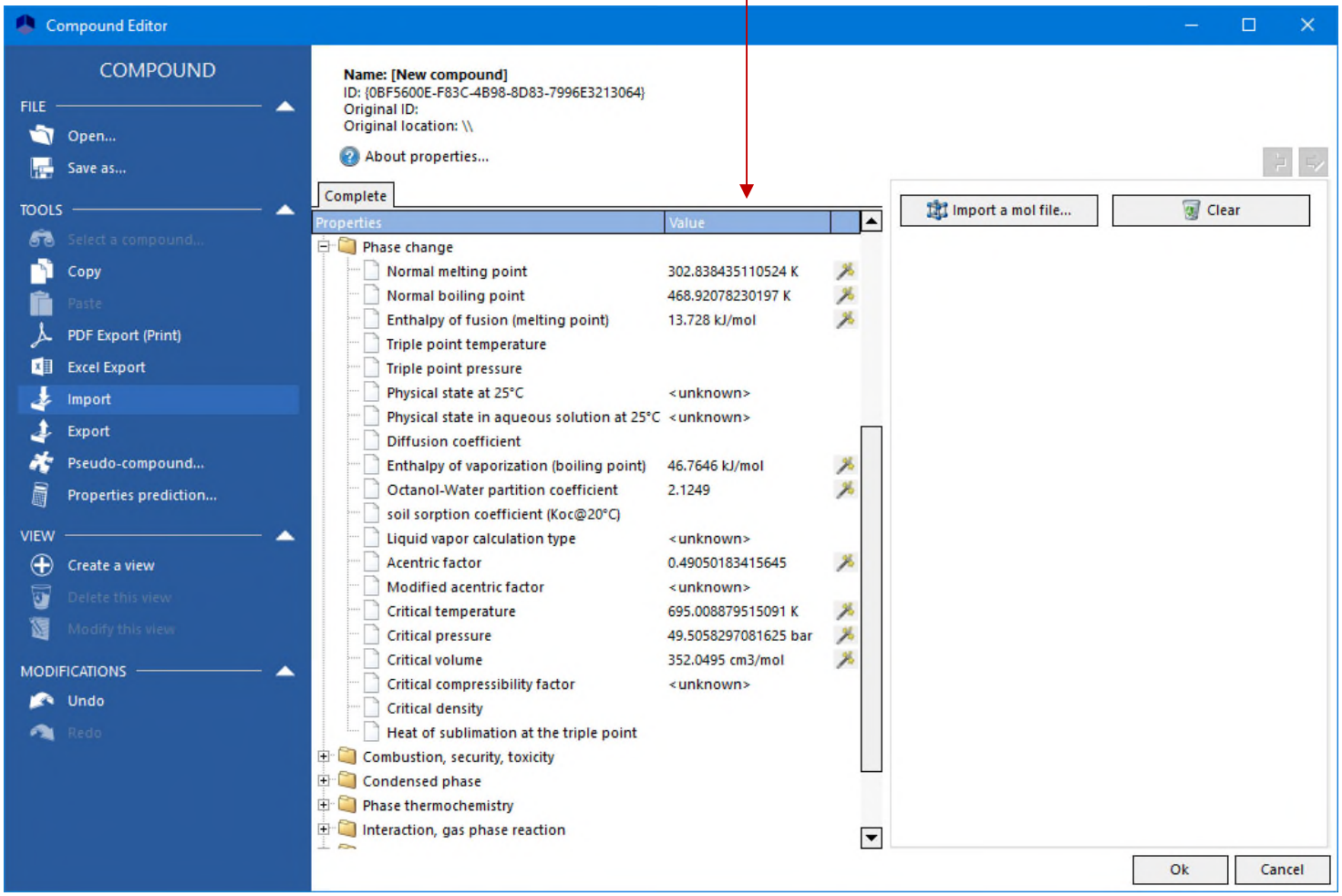
3. Allows to use for the calculations predicted values instead of current values

Access to the help: description of all estimation methods

6. Use

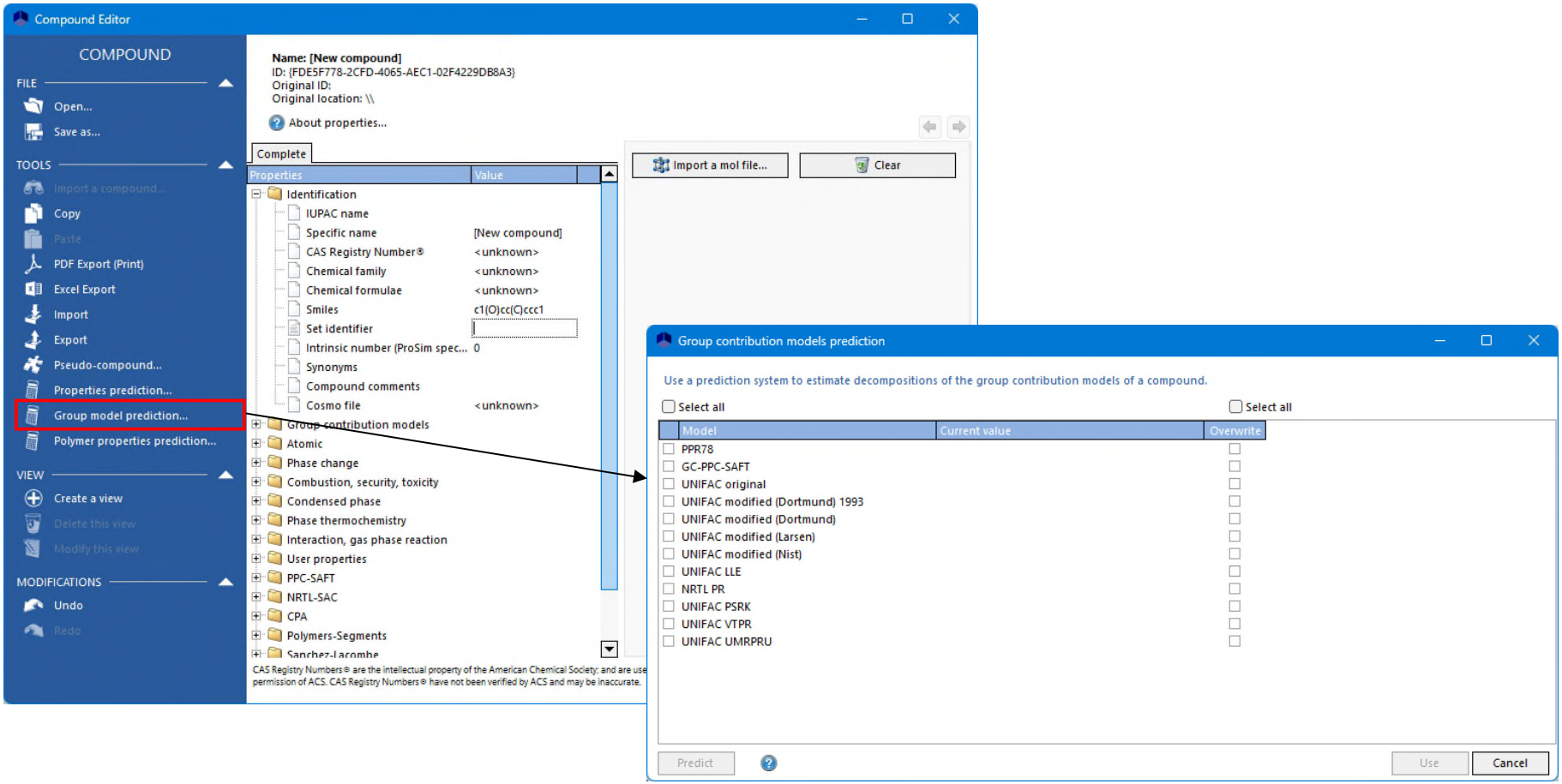
Step 3: Determine constant properties

Constant properties have been estimated by predictive methods from the SMILES of the molecule



Step 4: Decomposition into functional sub-groups

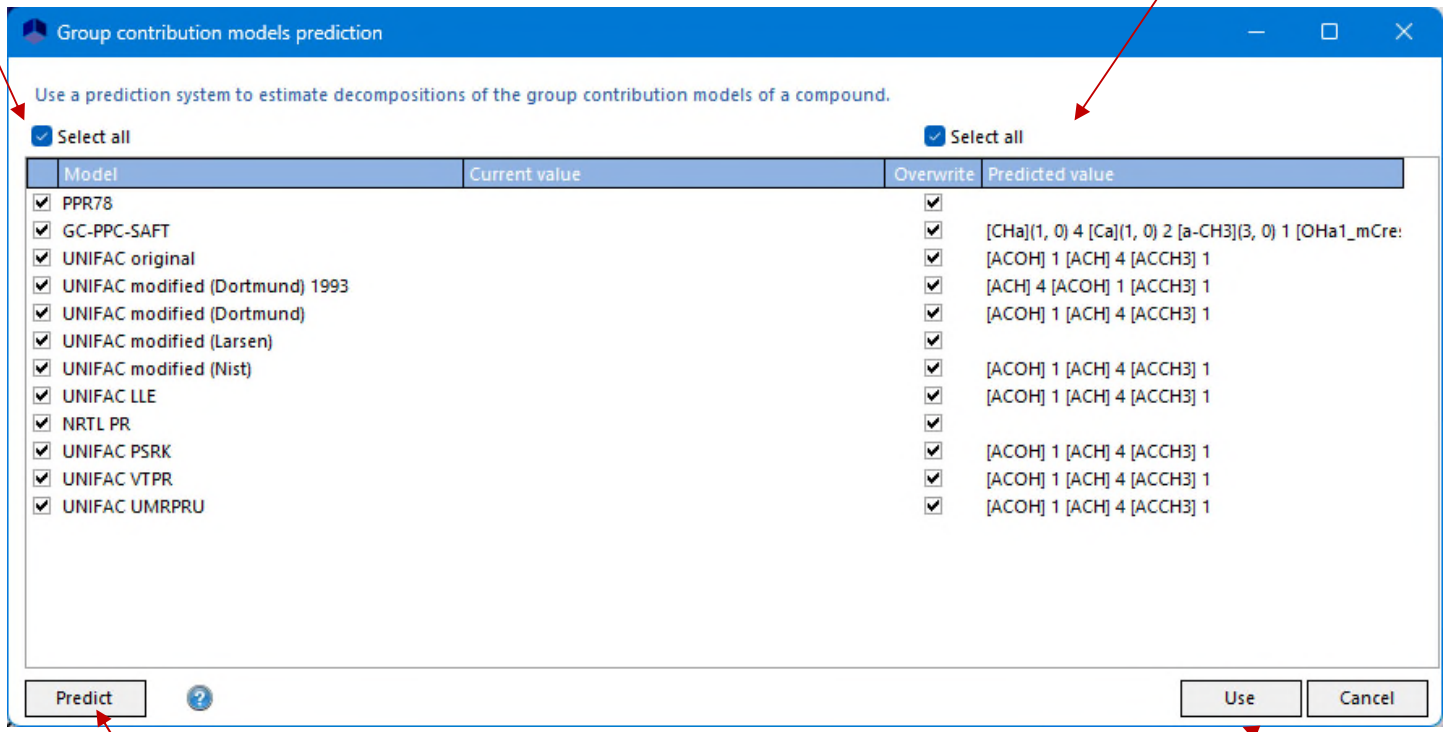
The use of a predictive thermodynamic model based on group contribution (UNIFACs, PPR78…) requires the knowledge of molecule decompositions in functional sub-groups



Step 3: Determine constant properties

1. Select all
(or only some models)

3. Select all
(or only some models)



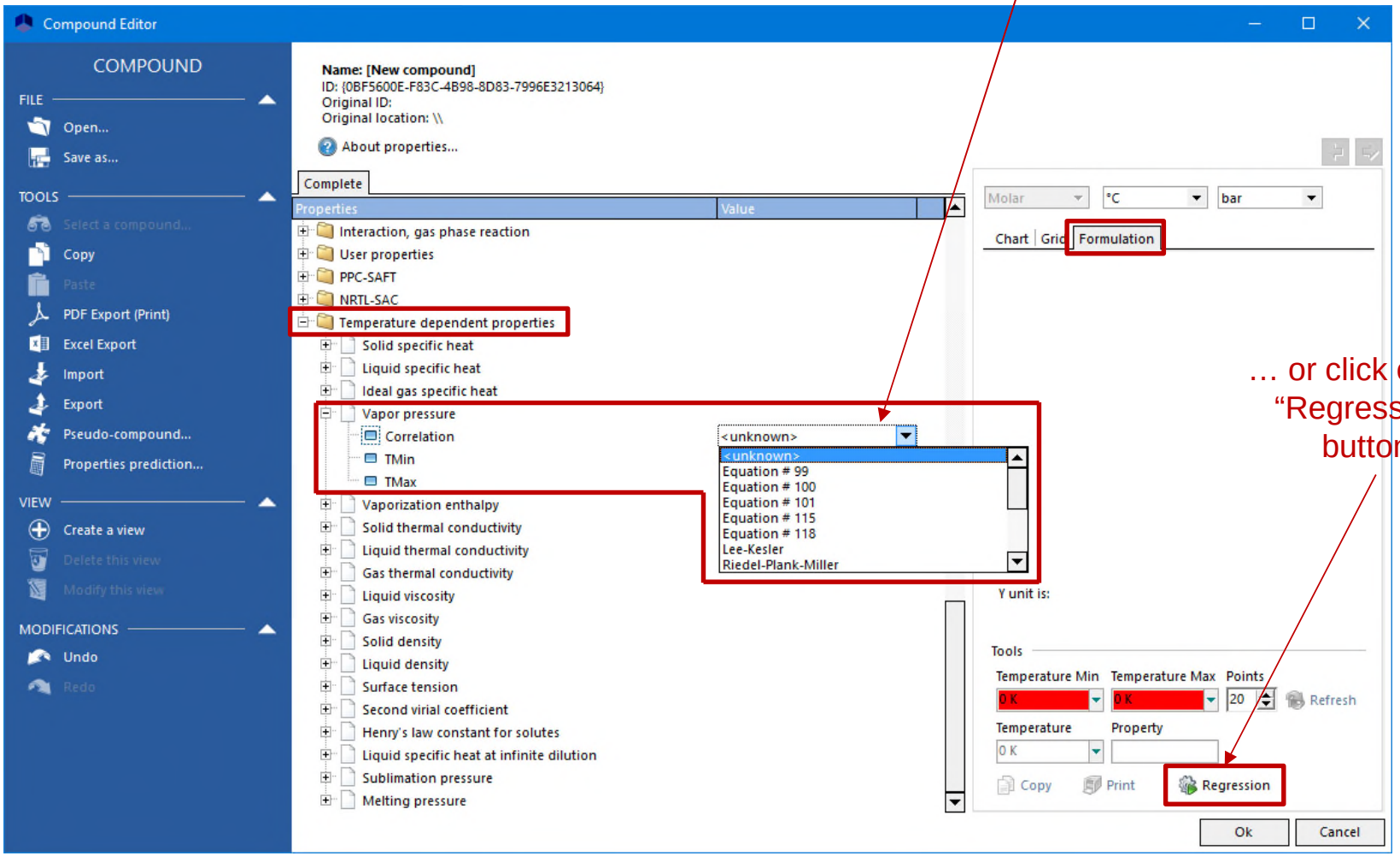
2. Click on the button allowing automatic decomposition of the molecule from its SMILES

4. Use

The automatic decomposition can fail if the molecule cannot be decomposed in the sub-groups available in the chosen group contribution model

Step 5: Temperature dependent properties

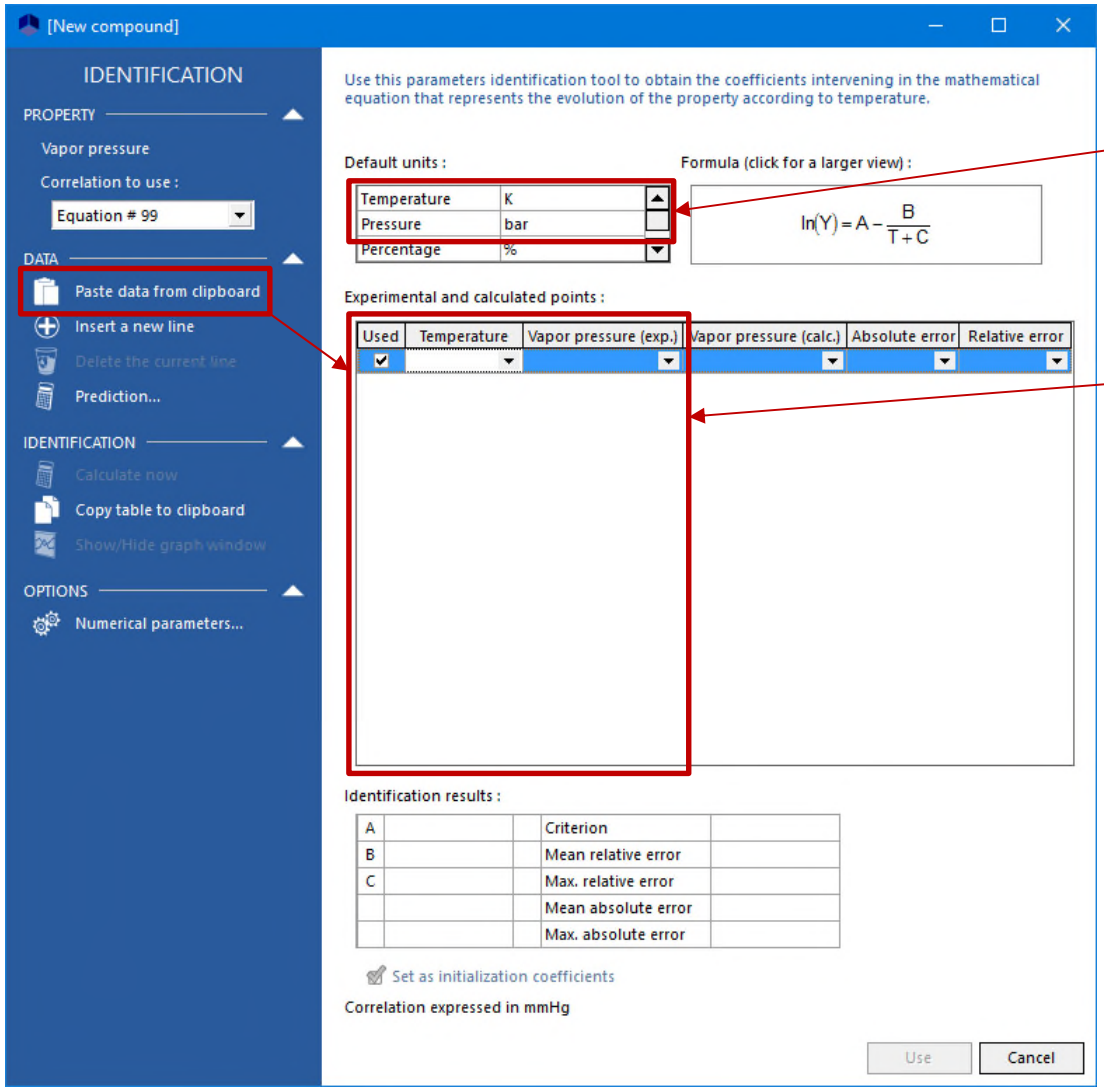
For temperature dependent properties, choose a correlation if it is known…



… or click on the "Regression" button

Step 5: Temperature dependent properties

If experimental data is available:



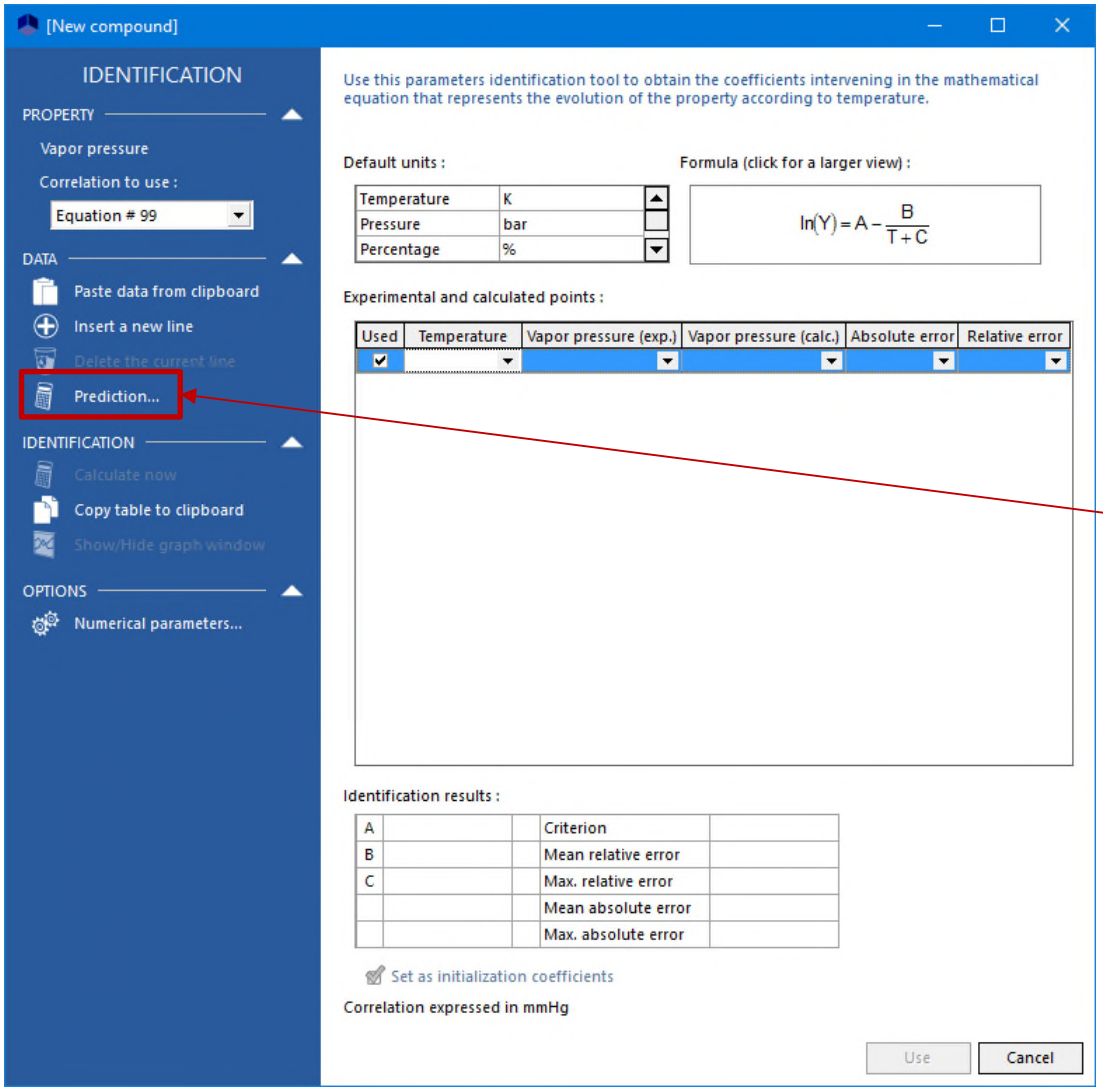
1. Select the units for the temperature and the property to be regressed

2. Copy/paste the table of experimental values temperature/property (e. g. from Excel)

⚠ Do not use "CTRL + V" to paste experimental values but the “Paste data from clipboard” button

Step 5: Temperature dependent properties

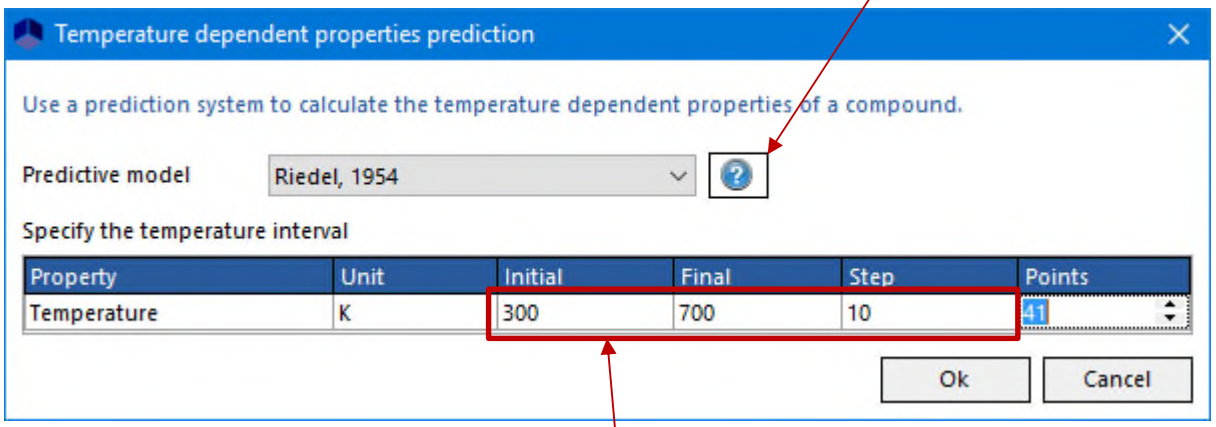
If no experimental data is available:



Click on the “Prediction…” button (only available if the SMILES has been provided)

Step 5: Temperature dependent properties

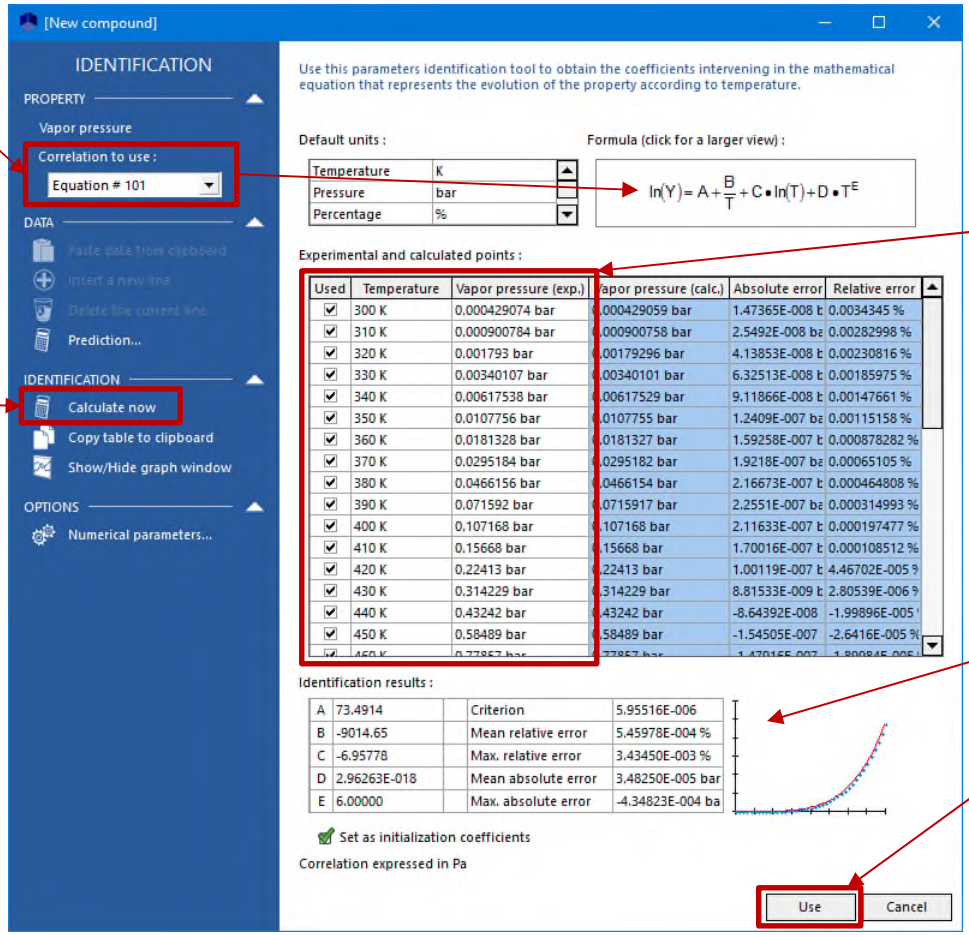
Generation of pseudo-experimental data estimated by predictive methods from the SMILES



Give the temperature range for the selected property
(e. g., for vapor pressure,
from the normal melting temperature to the critical temperature)
and the step of calculation to generate the expected number of points

Step 5: Temperature dependent properties

2. Select the correlation to be used for the regression



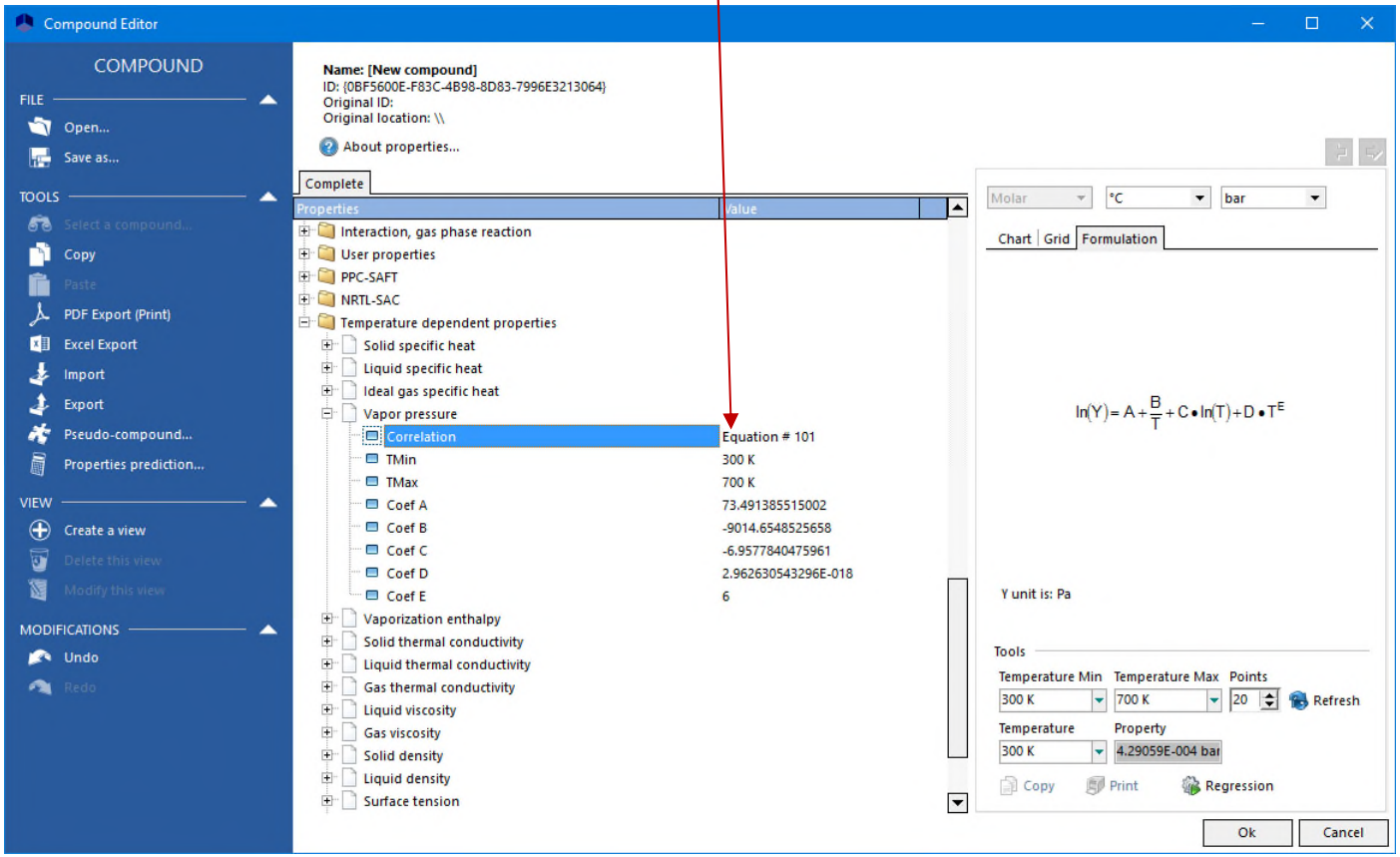
1. Data generated by the prediction tool

3.Click on “Calculate”

4. Verify the results of the regression, then click on “Use”

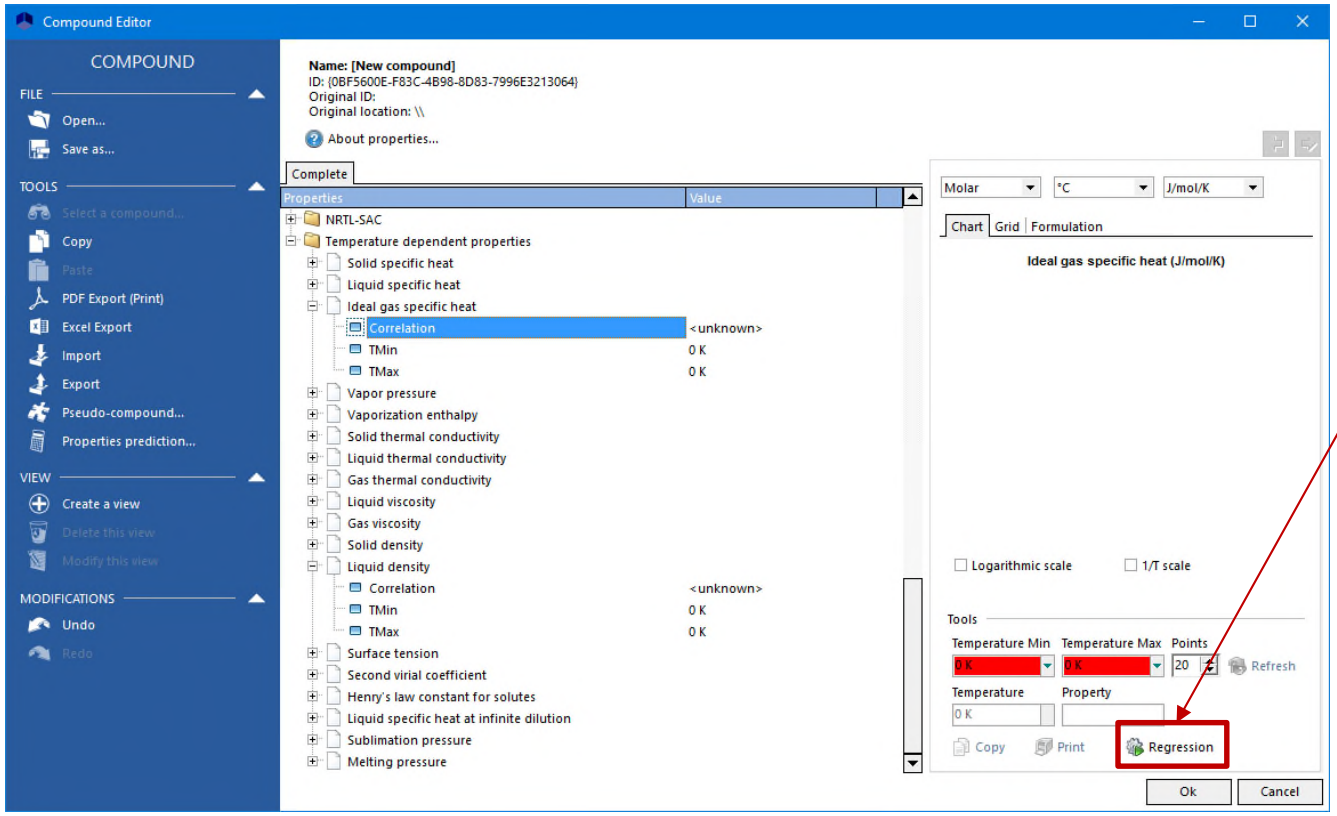
Step 5: Temperature dependent properties

Results of the regression of a temperature dependent property



Step 5: Temperature dependent properties

Renew the operation for the other temperature dependent properties (with a correlation, by regression from experimental data or estimated with the knowledge of the SMILES)



For the selected property, click on “Regression”. Generation of pseudo-experimental data from the SMILES is available for the following properties:

- *Vapor pressure*
- *Ideal gas specific heat*
- *Liquid density*
- *Liquid viscosity*
- *Surface tension*

Conclusion

The properties of a compound that is not available in databases:

- Constant
- Decomposition in functional sub-groups
- Temperature dependent

can be given by the user or estimated with predictive methods from the knowledge of the SMILES of the molecule.

The required properties to create a compound depend on the type of thermodynamic calculation (equilibrium, transport properties…)
and the choice of the thermodynamic model to represent the studied system (cf. help on thermodynamic models to know required pure component properties according to the chosen model)

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