

Predict Mix



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1 Introduction

DDB Predict Mix is a program to calculate different data types by a large variety of models.

1.1 Supported Data Types

DDB Predict Mix can calculate the following data types:

1. Vapor Liquid Equilibria
 - a. 2/3 Flash
 - b. VLE (Vapor-Liquid Equilibrium)
 - c. Henry
 - d. Phase Envelope
2. Solubility
 - a. SCF (Solubility in supercritical fluids)
 - b. SLE (Solid-Liquid Equilibrium)
 - c. LLE (Liquid-Liquid Equilibrium)
3. Activity
 - a. ACT (Activity coefficients at given concentrations)
 - b. ACT_inf (Activity coefficients at infinite dilution)
 - c. ACT_inf_all (Activity coefficient of given components with a list of solvents at infinite dilution)
4. Excess Properties
 - a. HE (Excess enthalpy)
 - b. VE (Excess volume)
 - c. CPE (Excess heat capacity)

1.2 Supported Group Contribution Models

DDB Predict Mix supports group contribution models like UNIFAC, UNIFAC 2.0, Modified UNIFAC (Dortmund), Modified UNIFAC 2.0, NIST-modified UNIFAC, Modified UNIFAC (Lyngby).

1.3 Supported Cubic EOS Mixing Rules

DDB Predict Mix supports the cubic equation of state models Soave-Redlich-Kwong (SRK), Peng-Robinson (PR), Peng-Robinson 1978 (PR78) and Redlich-Kwong (RK).

As K_{ij} mixing rules, the quadratic mixing rule and Panagiotopoulos/Reid are supported. In this case, the following temperature function is used:

$$K_{ij}[K] = a_{ij} + b_{ij}T + c_{ij}T^2 + \frac{d_{ij}}{T} + \frac{e_{ij}}{T^2}$$

As g^E mixing rules Vidal, Tochigi, Michelsen, PSRK, VTPR and LCVM are supported. In this case, the following temperature function is used:

$$G_{ij} = \exp\left(-\frac{T_{ij}}{RT}\right)$$

$$T_{ij}[\text{cal/mol}] = a_{ij} + b_{ij}T + c_{ij}T^2 + \frac{d_{ij}}{T} + e_{ij}T \cdot \ln(T) + f_{ij}T^3$$

The supported g^E models for the mixing rule are NRTL, Wilson, UNIQUAC, NRTL (Vidal) and UNIQUAC (res.).

For Soave-Redlich-Kwong and Peng-Robinson the original alpha functions (using the acentric factor ω), Mathias-Copeman¹ and Twu-Bluck-Cunningham-Coon² are supported. The Stryjek-Vera³ alpha function is available for Peng-Robinson only.

1.4 Supported Group Contribution Equation of State Models

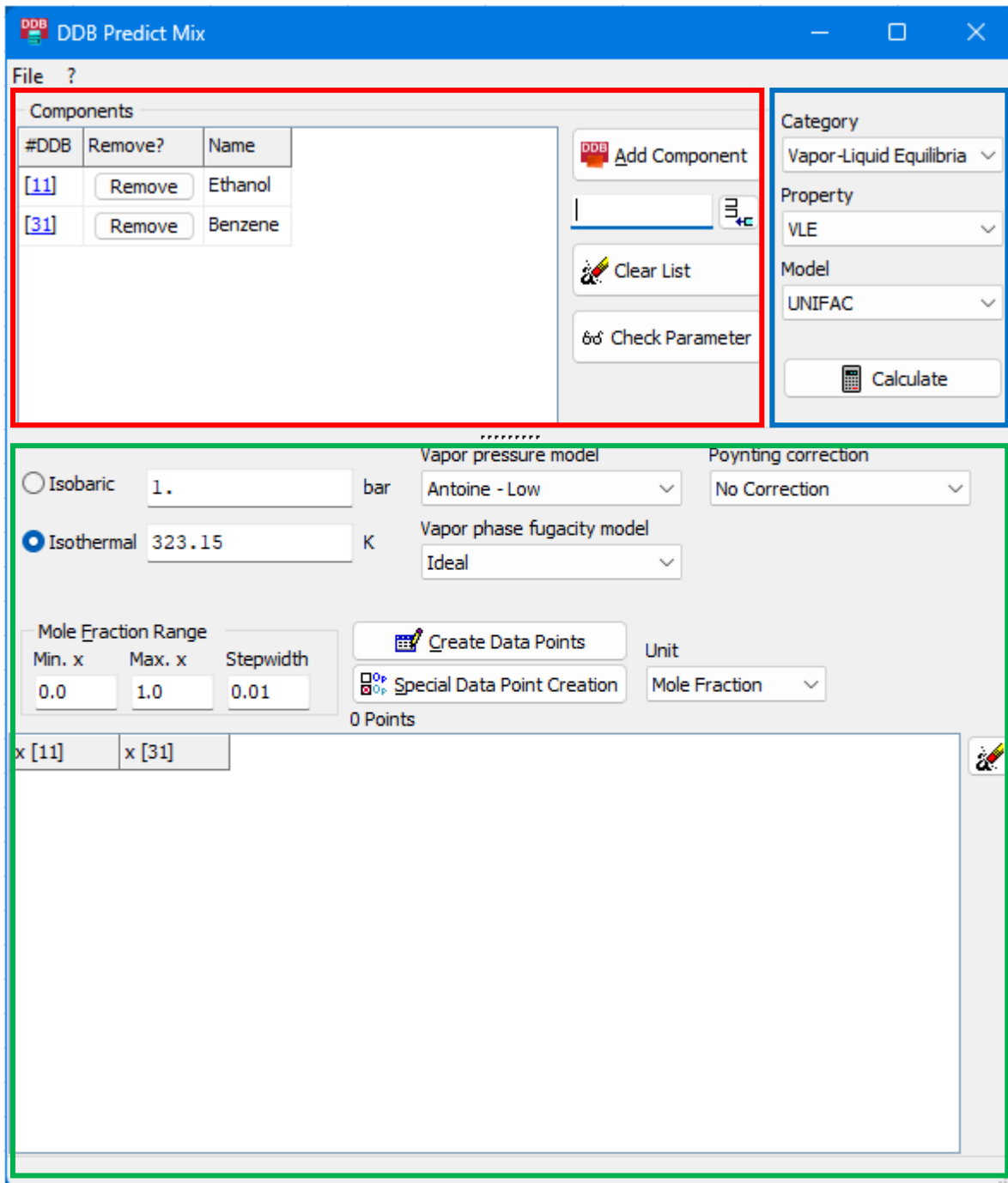
DDB Predict Mix supports the group contribution equation of states PSRK, PSRK2, PSRK 2.0 and VTPR.

¹ Mathias P.M., Copeman T.W., "Extension of the Peng-Robinson Equation of State to Complex Mixtures: Evaluation of the Various Forms of the Local Composition Concept", Fluid Phase Equilib., 13, 91-108, 1983

² Twu C.H., Bluck D., Cunningham J.R., Coon J.E., "A Cubic Equation of State with a New Alpha Function and a New Mixing Rule", Fluid Phase Equilib., 69, 33-50, 1991

³ Stryjek R., Vera J.H., "PRSV: An Improved Peng-Robinson Equation of State for Pure Compounds and Mixtures", Can.J.Chem.Eng., 64, 323-333, 1986

2 Menu




The menu has the following main parts:

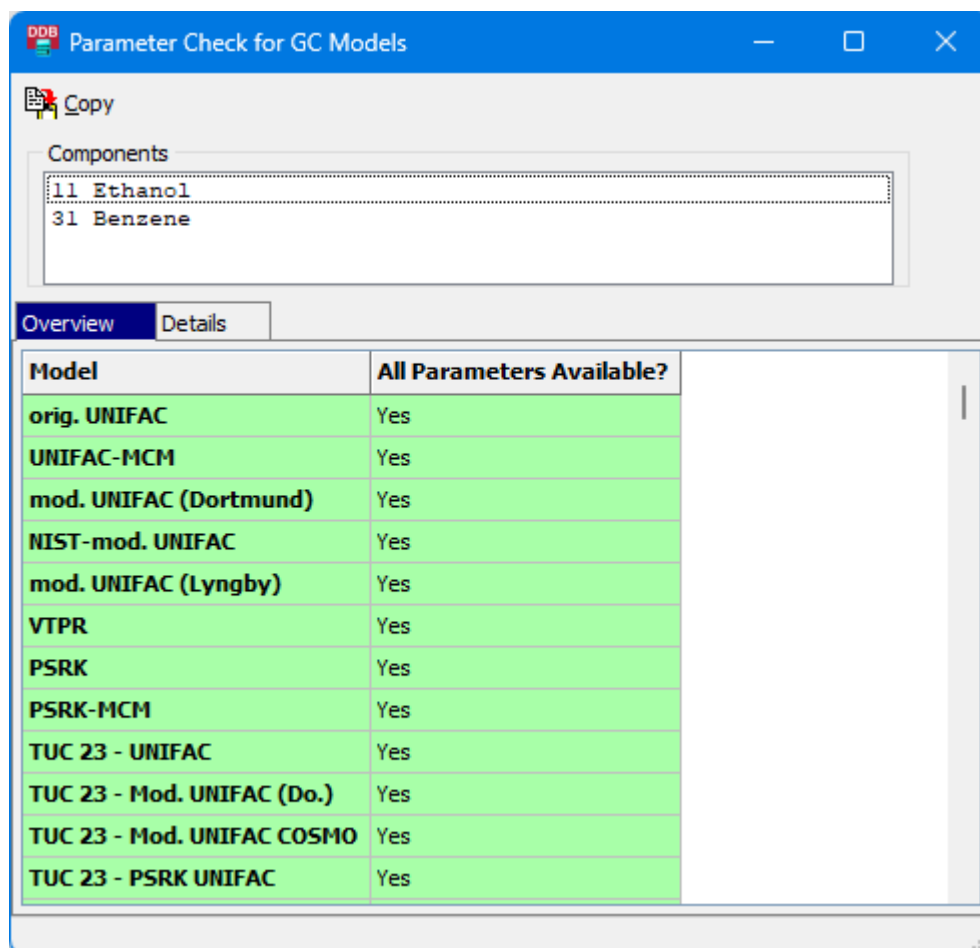
1. List of components (red)
2. Data type and model settings (blue)
3. Specific data type calculation options (green)
4. Splitter between red/blue and green area for enlarging the components grid

2.1 Component List

The list of components displays the current system, which should be calculated. New Components can be added by using the “Add Component” button. This will open DDB Components.

Components can also be added by typing the DDB numbers in the field beneath the “Add Component” button and confirming the numbers by using the  button. “Clear List” removes all components from the list. The “Remove” button deletes one specific component. A list of components can be loaded by the “Open System” option in the “File” menu. It is also possible to save the current system with the “Save System” option.

The “Check Parameters” button opens an extra menu for the parameter check. The “Overview” tab shows for which model all needed parameters are given for the defined component system. A more comprehensive view can be found in the “Details” tab.



The screenshot shows a window titled "Parameter Check for GC Models" with a "Copy" button and a list of components: "11 Ethanol" and "31 Benzene". Below the list are two tabs: "Overview" (selected) and "Details". The "Overview" tab displays a table with the following data:

Model	All Parameters Available?
orig. UNIFAC	Yes
UNIFAC-MCM	Yes
mod. UNIFAC (Dortmund)	Yes
NIST-mod. UNIFAC	Yes
mod. UNIFAC (Lyngby)	Yes
VTPR	Yes
PSRK	Yes
PSRK-MCM	Yes
TUC 23 - UNIFAC	Yes
TUC 23 - Mod. UNIFAC (Do.)	Yes
TUC 23 - Mod. UNIFAC COSMO	Yes
TUC 23 - PSRK UNIFAC	Yes

2.2 Data Type and Model Settings

The general options of the calculation are in the upper right corner of the menu. DDB Predict Mix is able to calculate a large amount of data types. So data types are categorized for reasons of clarity. After a suitable category is chosen, the user can select the right property from the menu. Further calculation options are given at the bottom of the menu after the property selection. The last dropdown menu allows the selection of the model.

Category
Vapor-Liquid Equilibria ▾

Property
2/3 Flash ▾

Model
PSRK ▾

The “Calculate” button starts the calculation. In a case of an EOS model selection a further menu for EOS options and parameter selection will open.

VLE Calculation by EOS

Components
11: Ethanol
31: Benzene

Equation of State
1 - Soave-Redlich-Kwong ▾

Mixing Rule
2 - gE-Vidal ▾

gE Model
4 - NRTL (Vidal) ▾

Alpha Function
1 - Mathias-Copeman ▾

Interaction Parameters

Binary Interaction Parameters: $(T_{ij} [\text{cal/mol}] = a_{ij} + b_{ij} \cdot T + c_{ij} \cdot T^2 + d_{ij}/T + e_{ij} \cdot T \cdot \ln(T) + f_{ij} \cdot T^3)$

Comp't 1	Comp't 2	a12	b12	c12	d12	e12	f12	g12	a21	b21	c21	Kij
11	31	52.043272	0	0	0	0	0	0	1501.6956	0	0	

OK Cancel

In this menu the Equation of State, the Mixing Rule, the gE Model and the Alpha Function can be selected. The Parameters can then be set by hand or by using the “Kij” button. This option allows parameters to select from the library or from a project file. If there are already recommended parameters in the library, they will be automatically loaded to the menu.

3 Calculation

DDB Predict Mix gives further calculation options for every property at the bottom of the menu.

3.1 Vapor-Liquid Equilibria

3.1.1 2/3 Flash

The 2/3 Flash program can calculate the phase split for a given feed concentration at the given temperature and pressure. This calculation needs an equation of state as basis model.

Temperature: 323 K
 Pressure Range [bar]: 0.4, 0.5, 0.01
 Flash Type: VL-Flash
 Constant Temperature
 Constant Pressure
 PSRK Volume Correction

Component	Mole Fractions
11	0.2
31	0.8

Current Sum: 1
 Type: Mole Fractions

The options on the top left allow defining a constant temperature or pressure and an associated temperature or pressure range. A vapor-liquid or a vapor-liquid-liquid flash can be selected with the “Flash Type” Combo box on the right. The box beneath activates the PSRK Volume correction. In the “Feed Compositions” box, the concentrations for the calculation are stored, either in mole fractions or in weight fractions. Further columns are added by using the “Enter” key in the last row.

Result

The result table starts with small list of the used components. This is followed by a model dependent list of constants and parameters, which are used for the calculation.

T [K] = 323 P [bar] = 0.44										
No.	#DDB	z(i)-Feed	Given Feed N(i)-Feed	x(i)-Phase 1	N(i)-Phase 1	Liquid phase phi(i)-Phase 1	y(i)-Phase 2	N(i)-Phase 2	Vapor phase phi(i)-Phase 2	Fug(i) [bar]
1	11	2.000000e-01	2.000000e-01	6.549702e-02	8.334671e-03	3.319941e+00	2.196115e-01	1.916653e-01	9.901406e-01	9.567635e-02
2	31	8.000000e-01	8.000000e-01	9.345030e-01	1.189180e-01	8.226038e-01	7.803885e-01	6.810820e-01	9.850551e-01	3.382393e-01
N [mol]				1		0.127253			0.872747	
M [G]				71.7047		9.67309			62.0316	
V [L/mol]						0.0994136			60.1793	
Z = PV/RT						0.00162887			0.986024	
Rho [g/ccm]						0.764632			0.00118107	
h-h0 [J/mol]						-32797.7			-104.464	
s-s0 [J/mol/K]						-100.677			-0.207624	

The result table shows detailed information about the used feed concentration and the resulting phases at the given temperature and pressure. The table shows the state of the given phases and gives information about concentration, amount of the component and the fugacity coefficients. Further information is given below the small tables. The following tables explain the abbreviations.

Abbreviations in the table:

Short Term	Description
i	Component (numbering order from top to bottom as in the main form's component list)
z(i)	Mole fraction of component I in the feed
x(i)	Mole fraction of component I in the liquid phase
y(i)	Mole fraction of component I in the vapor phase
F	Total feed (1 mole)
N(i)	Total number of moles of component I in the described phase (Total feed 1 mole)
phi(i),L	Liquid phase fugacity coefficient
phi(i),V	Vapor phase fugacity coefficient
Fug(i)	Fugacity $f = \Phi_{L,i} \cdot x_i \cdot P$ $f = \Phi_{V,i} \cdot y_i \cdot P$

Abbreviations on the edge of the table:

Short Term	Description
N	Amount of substance of the phase (complete, liquid phase, vapor phase)
M	Mass (complete, liquid phase, vapor phase)
V	Volume (liquid phase, vapor phase)
Z	Compressibility (liquid phase, vapor phase)
V (Penelouxcorr.)*	Volume (liquid phase, vapor phase)
Rho (Penelouxcorr.)*	Density (liquid phase, vapor phase)
h-h0	Real part of enthalpy (liquid phase, vapor phase, complete system)
s-s0	Real part of entropy (liquid phase, vapor phase, complete system)

*"Penelouxcorr." means that the Peneloux correction for the density was taken into account.

3.1.2 VLE

A constant pressure or a constant temperature can be specified for the VLE calculation. It is also possible to define the liquid concentrations for the calculation. These points can either be created by using the “Create Data Points” or “Special Data Point Creation” button. The first option uses the Mole Fraction range and creates with the limits and step width on the left side the desired concentrations. The second option uses an extra menu with more options for ternary and higher systems. This menu also allows creating concentrations by hand. If no concentrations are given in the feed, the program will create concentrations with the help of the first option. If a group contribution model is chosen, further options for the vapor pressure model, the vapor phase fugacity model and the Poynting correction appear.

The screenshot shows the VLE calculation settings. Under 'Isothermal', the temperature is 323.15 K. The 'Vapor pressure model' is 'Antoine - Low' and 'Poynting correction' is 'No Correction'. The 'Vapor phase fugacity model' is 'Ideal'. The 'Mole Fraction Range' is defined by Min. x: 0.0, Max. x: 1.0, and Stepwidth: 0.1. There are buttons for 'Create Data Points' and 'Special Data Point Creation'. A table shows the generated mole fractions for three components: x [11], x [31], and x [161]. The first row is 0.0, 0.0, 1.0 and the second row is 0.0, 0.1, 0.9. The total number of points is 66.

x [11]	x [31]	x [161]
0.0	0.0	1.0
0.0	0.1	0.9

Vapor phase fugacity model

DDB Predict Mix supports an ideal vapor phase but automatically switches to the Marek/Standart method for an internally stored list of carboxylic acids considering the vapor phase association.

The other methods include different cubic equations of state with the quadratic mixing rule and the Hayden-O-Connell method.

Vapor pressure model

The following pure component vapor pressure equations (see the PCPEquationFit documentation for the equation details) are supported:

1. Antoine – Low: This option searches the list of available Antoine parameter sets for that one which has the lowest lower validity range (this option was implemented to mimic the behavior of RecVal, which uses a low temperature and a high temperature set of Antoine parameters).
2. DIPPR 101 equation
3. Wagner equation (2.5-5 form)
4. Extended Antoine (Aspen)

Poynting Correction

The Poynting correction needs pure component densities resp. volumes v_i .

$$Poy_i = \exp \frac{v_i(P - P_i^s)}{RT}$$

DDB Predict Mix supports:

1. Densities calculated with the DIPPR 105 equation. These aren't original DIPPR parameters. The parameters are regressed by DDBST personnel with the help of the DDB pure component properties data bank (“PCP Equation Fit” program).

2. Densities by the Yen/Woods⁴ correlation.

Result

The result table starts with a small list of the used components. This is followed by a model dependent list of constants and parameters, which are used for the calculation. The results are given after that in table form.

I`x	T [K]	P [kPa]	x1 [mol/mol]	x2 [mol/mol]	y1 [mol/mol]	y2 [mol/mol]	Act.C.1[-]	Act.C.2[-]	phi.L.1[-]
1	323.150	36.362	0.00000	1.00000	0.00000	1.00000	7.52842	1.00000	6.08779
2	323.150	38.113	0.01000	0.99000	0.05452	0.94548	7.01718	1.00035	5.41398
3	323.150	39.616	0.02000	0.98000	0.09817	0.90183	6.56099	1.00137	4.87017
4	323.150	40.910	0.03000	0.97000	0.13380	0.86620	6.15221	1.00303	4.42238
5	323.150	42.029	0.04000	0.96000	0.16336	0.83664	5.78447	1.00527	4.04749
6	323.150	42.999	0.05000	0.95000	0.18823	0.81177	5.45243	1.00807	3.72922
7	323.150	43.842	0.06000	0.94000	0.20939	0.79061	5.15160	1.01140	3.45580
8	323.150	44.576	0.07000	0.93000	0.22758	0.77242	4.87816	1.01525	3.21851
9	323.150	45.218	0.08000	0.92000	0.24336	0.75664	4.62886	1.01957	3.01072
10	323.150	45.780	0.09000	0.91000	0.25717	0.74283	4.40091	1.02436	2.82736
11	323.150	46.273	0.10000	0.90000	0.26933	0.73067	4.19194	1.02961	2.66442

The table contains the following abbreviations.

Column	Description
I`x	Sequential number
T	Temperature
P	Pressure
x1	Liquid mole fraction of component 1 (carbon dioxide in this example)
y1	Vapor mole fraction of component 1
Act. C.1	Activity coefficient of component 1
phi. L.1	Liquid fugacity coefficient for component 1
phi. V. 1	Vapor fugacity coefficient for component 1
Fug 1	Fugacity for component 1
vv	Vapor volume
vl	Liquid volume
vE	Excess volume
hE	Excess enthalpy

The output is finished if a critical point has been identified or the complete composition range has been calculated. If an azeotropic point has been identified it will be displayed in the table. Beside these tables, several plots are generated. These plots can be printed, saved and copied to the Windows clipboard.

⁴ Yen L. C., Woods S. S., "A Generalized Equation for Computer Calculation of Liquid Densities", AIChE J., 12(1), 95-99, 196

3.1.3 Henry

The Henry calculation only works for binary systems.

For the GLE (Gas-Liquid Equilibrium) calculation, it is necessary to define which component is the liquid solvent. In addition, a vaporous component that dissolves in the solvent phase must be defined. At the bottom of the menu, the user defines a temperature range for the calculation.

Result

The results are shown after the component and parameter list.

Calculation of Henry coefficients
 Solute: 1050 Carbon dioxide
 Solvent: 31 Benzene

T [K]	H12 [bar]	Psat2 [bar]	vL [1/mol]	vV [1/mol]
298.00	94.1085	0.1525	0.09828	161.364
303.00	101.7870	0.1868	0.09881	133.816
308.00	109.6949	0.2273	0.09935	111.657
313.00	117.7667	0.2748	0.09991	93.714
318.00	125.9718	0.3303	0.10049	79.091
323.00	134.2804	0.3947	0.10108	67.102

With the following abbreviations

Column	Description
T	Temperature
H12	Henry coefficient
PSAT2	Saturated vapor pressure of the solvent
VL	Liquid volume
VV	Vapor volume

Beside this table, several plots are generated. These plots can be printed, saved and copied to the Windows clipboard.

3.1.4 Phase Envelope

The Phase Envelope calculation works only for models with an Equation of State.

Composition

Component	Mole Fractions
11	0.1
31	0.1
1050	0.8

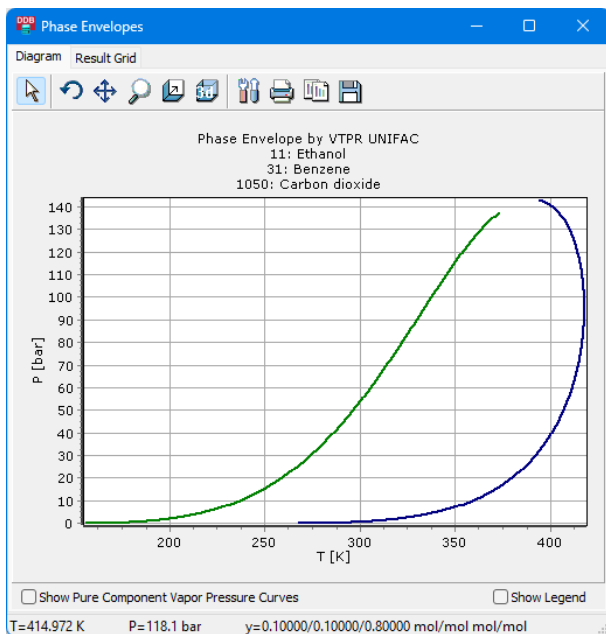
Current Sum: 1

Type: Mole Fractions

The constant concentration for the liquid and vapor phase is defined in the “Composition” box as either mole fractions or weight fractions.

Result

The results are presented in a diagram. It is possible to add the pure vapor pressure curves and the legend by the options at the bottom of the diagram. The exact calculated points can be found in the “Result Grid” Tab. Temperature and pressure are T and P, x1 and y1 are the liquid and vapor phase concentrations of component 1. The volume is represented by v.



	T [K]	x1 [mol/mol]	P [bar]	y1 [mol/mol]	v vapor [dm ³ /mol]	v liq
x	156.1640	0.10000	0.1000	0.00000	129.4196	0.03
x	178.6776	0.10000	0.6000	0.00000	24.4184	0.04
x	188.2237	0.10000	1.1000	0.00000	13.9115	0.04
x	194.7683	0.10000	1.6000	0.00000	9.8215	0.04
x	199.8710	0.10000	2.1000	0.00000	7.6250	0.04
x	204.1079	0.10000	2.6000	0.00001	6.2475	0.04
x	207.7608	0.10000	3.1000	0.00001	5.2998	0.04
x	210.9900	0.10000	3.6000	0.00001	4.6065	0.04
x	213.8963	0.10000	4.1000	0.00002	4.0763	0.04
x	216.5472	0.10000	4.6000	0.00002	3.6572	0.04
x	218.9905	0.10000	5.1000	0.00002	3.3173	0.04
x	221.2614	0.10000	5.6000	0.00003	3.0359	0.04
x	223.3864	0.10000	6.1000	0.00003	2.7989	0.04
x	225.3863	0.10000	6.6000	0.00004	2.5964	0.04
x	227.2775	0.10000	7.1000	0.00004	2.4213	0.04
x	229.0732	0.10000	7.6000	0.00005	2.2684	0.04
x	230.7844	0.10000	8.1000	0.00005	2.1337	0.04
x	232.4302	0.10000	8.6000	0.00006	2.0138	0.04

3.2 Solubility

3.2.1 SCF

The SCF (Solubility in supercritical fluid) calculation needs an Equation of State as basis model.

On the right side, the calculation temperature is set. The first combo box on the left side specifies the supercritical fluid as solvent for the extraction. Below that, the solute and its associated solid volume and vapor pressure equation are defined. Additionally, a co-solvent can be defined with its concentration in the solvent. At the bottom of the menu, the source of sublimation vapor pressure can be set.

Result

The results are shown after the component and parameter list.

Solubility of Carbon dioxide
in supercritical Naphthalene
Co-solvent: Ethanol

Solid volume of solute: 0.1119 dm³/mol

Temperature: 323 K

P[bar]	vV[dm ³ /mol]	y(2)	log(y2)	PHI(2)	POYN(2)	y(1)	y(3)
2.00	13.2935	5.37504733e-04	-3.26962	0.93223	1.00837	0.899462	1.00000000e-01
4.00	6.5790	2.90962049e-04	-3.53616	0.86828	1.01681	0.899709	1.00000000e-01
6.00	4.3402	2.10224811e-04	-3.67732	0.80787	1.02532	0.899790	1.00000000e-01
8.00	3.2204	1.71065323e-04	-3.76684	0.75083	1.03391	0.899829	1.00000000e-01
10.00	2.5480	1.48652297e-04	-3.82783	0.69702	1.04256	0.899851	1.00000000e-01
12.00	2.0995	1.34722540e-04	-3.87056	0.64627	1.05129	0.899865	1.00000000e-01

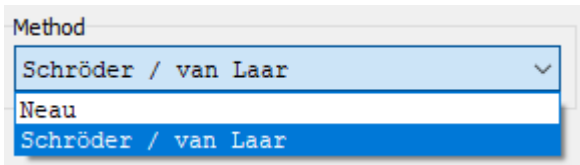
With the following abbreviations

Column	Description
P	Pressure
VV	Vapor volume
Y2	Vapor mole fraction of component 2
PHI(2)	Fugacity coefficient of component 2
POYN	Poynting factor

Beside this table, a diagram is created which shows the logarithmic concentration of the solute against the pressure. This graphic can be saved and copied

3.2.2 SLE

For the SLE (Solid-Liquid Equilibrium) a calculation method has to be chosen from the “Method” Combo Box



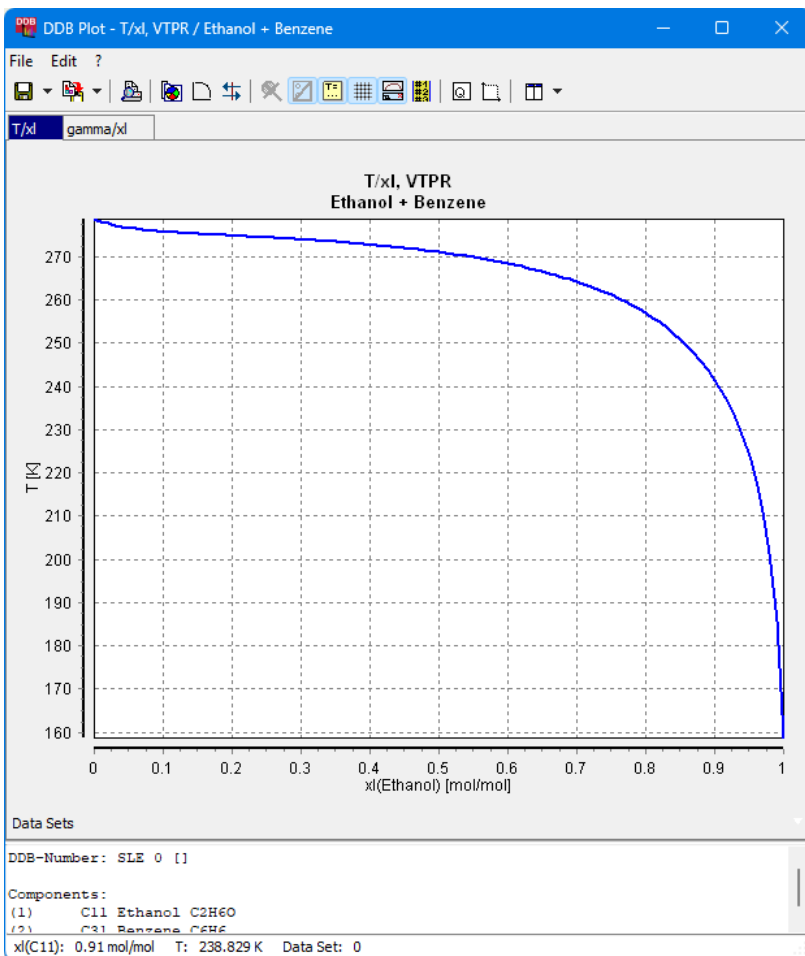
The calculation concentration can be set at the bottom of the menu. The options are similar to the VLE calculation.

Result

The results are shown after the component and parameter list (e.g. Ethanol + Benzene).

T [K]	x1 [1]	x1 [2]	gamma [1]	gamma [2]
278.68	0.0000	1.0000	23.0324	1.0000
278.10	0.0100	0.9900	18.5506	1.0011
277.64	0.0200	0.9800	15.3636	1.0041
277.26	0.0300	0.9700	13.0161	1.0085
276.95	0.0400	0.9600	11.2343	1.0141

T is the temperature and x1[1] is the liquid phase concentration of component 1. Additionally, the results are shown as diagram.



This diagram can be printed, saved or copied. It is also possible to edit the chart.

3.2.3 LLE

The LLE (Liquid-Liquid Equilibrium) calculation works only for binary systems. A temperature range can be set in the menu.

Temperature [K]

Start	End	Step
298	323	5

Pressure [bar]

1.

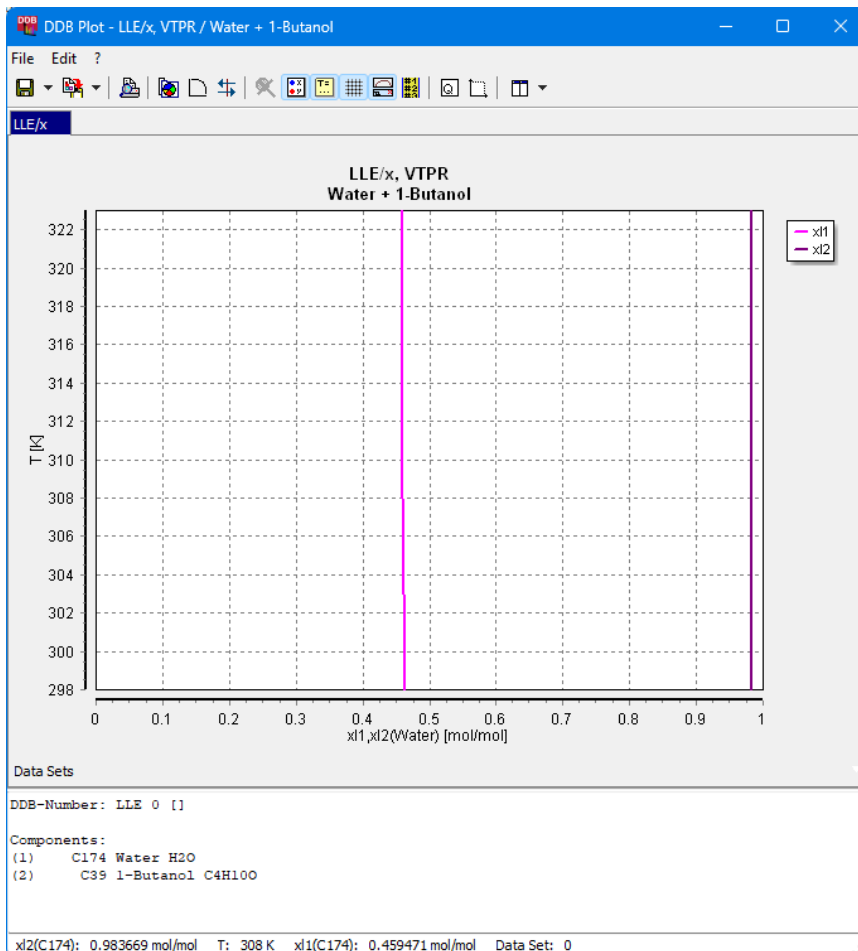
The pressure is only relevant for calculation with Equation of States.

Result

The results are shown after the component and parameter list (e.g., Water + 1-Butanol).

T [K]	P [bar]	x111	x112	x121	x122
298.00	1.00	0.46371	0.53629	0.98383	0.01617
303.00	1.00	0.46104	0.53896	0.98377	0.01623
308.00	1.00	0.45944	0.54056	0.98367	0.01633
313.00	1.00	0.45883	0.54117	0.98353	0.01647
318.00	1.00	0.45911	0.54089	0.98336	0.01664
323.00	1.00	0.46021	0.53979	0.98316	0.01684

Temperature and pressure are T and P, x112 is the concentration in phase 1 of component 2. Additionally, the results are shown as diagram.

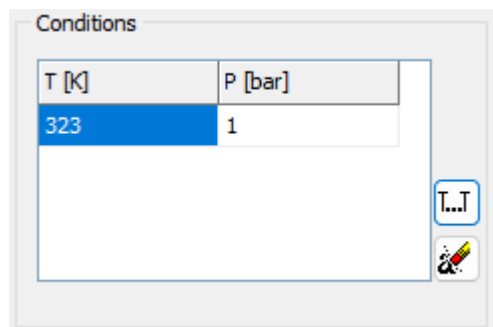


This diagram can be printed, saved or copied. It is also possible to edit the chart.

3.3 Activity

3.3.1 ACT

The ACT (Activity) calculation determines the activity coefficients for given temperatures, pressures and concentrations.



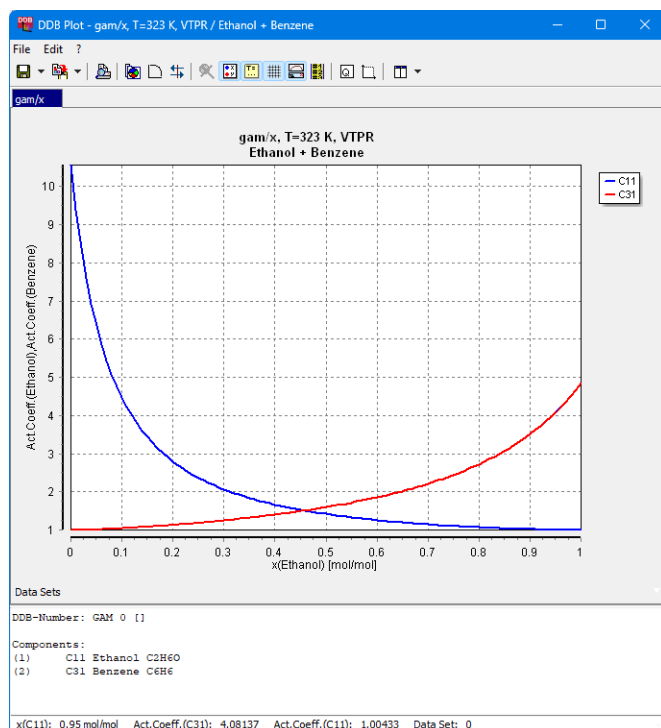
The “Condition” box contains the given calculation temperature and pressure. The concentrations are defined similar to the VLE calculation.

Result

The results are shown after the component and parameter list (e.g., Ethanol + Benzene).

T [K]	P [bar]	x1	x2	gamma1	gamma2
323.00	1.00	0.00000	1.00000	10.56279	1.00000
323.00	1.00	0.01000	0.99000	9.37274	1.00059
323.00	1.00	0.02000	0.98000	8.40178	1.00225
323.00	1.00	0.03000	0.97000	7.59809	1.00483
323.00	1.00	0.04000	0.96000	6.92433	1.00822
323.00	1.00	0.05000	0.95000	6.35310	1.01231
323.00	1.00	0.06000	0.94000	5.86394	1.01704

Temperature and pressure are T and P, x1 is the concentration of component 1 and gamma1 is the activity coefficient of component 1. Additionally, the results are shown as diagram.



This diagram can be printed, saved or copied. It is also possible to edit the chart.

3.3.2 ACT_inf

The ACT_inf property calculates the activity coefficients of two components at infinite dilution in each other.

Temperature [K]

Start	End	Step
298	323	5

Pressure [bar]

1.

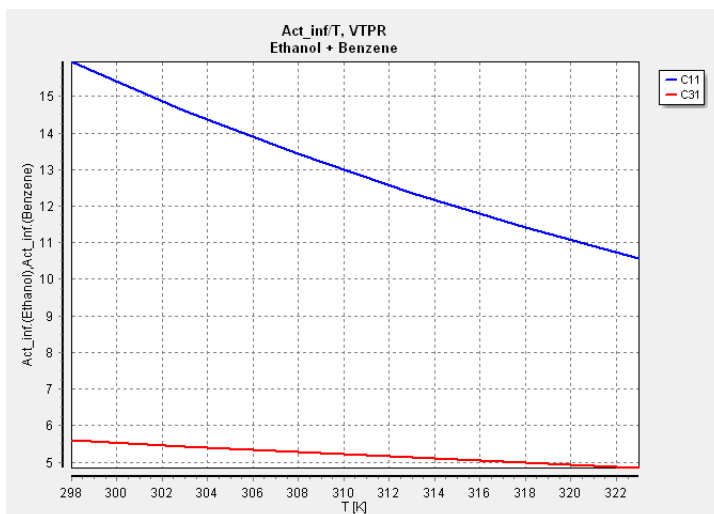
The temperature range has to be set in the menu for the calculation.

Result

The results are shown after the component and parameter list (e.g., Ethanol + Benzene).

T [K]	P [bar]	Actinf1	Actinf2
298.00	1.00	15.95177	5.60115
303.00	1.00	14.61196	5.43918
308.00	1.00	13.42161	5.28256
313.00	1.00	12.36079	5.13097
318.00	1.00	11.41263	4.98414
323.00	1.00	10.56279	4.84182

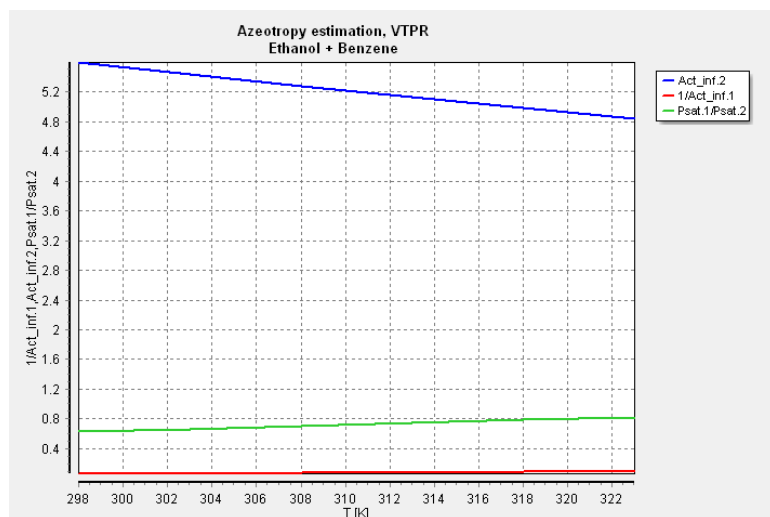
T is the temperature and P is the pressure. Actinf1 is the activity coefficient of component 1 in infinite dilution in component 2. Additionally, there are two further diagrams. The first shows the activity coefficient against the temperature.



The second graphic is used for azeotropy estimation. Actinf2 and $1/\text{Actinf1}$ and the quotient of the vapor pressure of component 1 and 2 are shown in the graphic. If the green line is between the blue and red line azeotropic behavior is given. If the green line is above or below both other lines the system is zeotropic. If the blue line is above the red line the system shows a positive azeotrope and if the red line is above the blue line the system shows a negative azeotrope.

$$\text{Positive Azeotrope } \gamma_2^\infty > \frac{P_1^S}{P_2^S} > \frac{1}{\gamma_1^\infty}$$

$$\text{Negative Azeotrope } \gamma_2^\infty < \frac{P_1^S}{P_2^S} < \frac{1}{\gamma_1^\infty}$$



3.3.3 ACT_inf_all

The ACT_inf_all property allows the calculation of the activity coefficients of the system components at infinite dilution in single solvents from a given list. The calculation is also done vice versa.

Temperature [K] Use only components from list

Pressure [bar] Check Azeotropy Criterion

The calculation temperature and pressure can be set on the left side of the menu. The pressure is only used for calculation with an Equation of State. Normally, the calculation is done for all components of the DDB. This is very time consuming. A list of components can be loaded with the -button. It is also possible to choose a list of solvents with DDB Components by using the -button. The -button opens an extra menu. In this menu, a range of components can be selected by using the lowest and highest DDB Number. If the “Check Azeotropy Criterion” is activated, the pure component vapor pressures and an extra azeotropy criterion are calculated in addition to the activity coefficients.

Result

The results are shown in a form of a table for every solvent. Only successful calculations of the activity coefficient are shown.

Model: mod. UNIFAC (Dortmund)

List of components:

No.	#DDB	Name
(1)	11	Ethanol

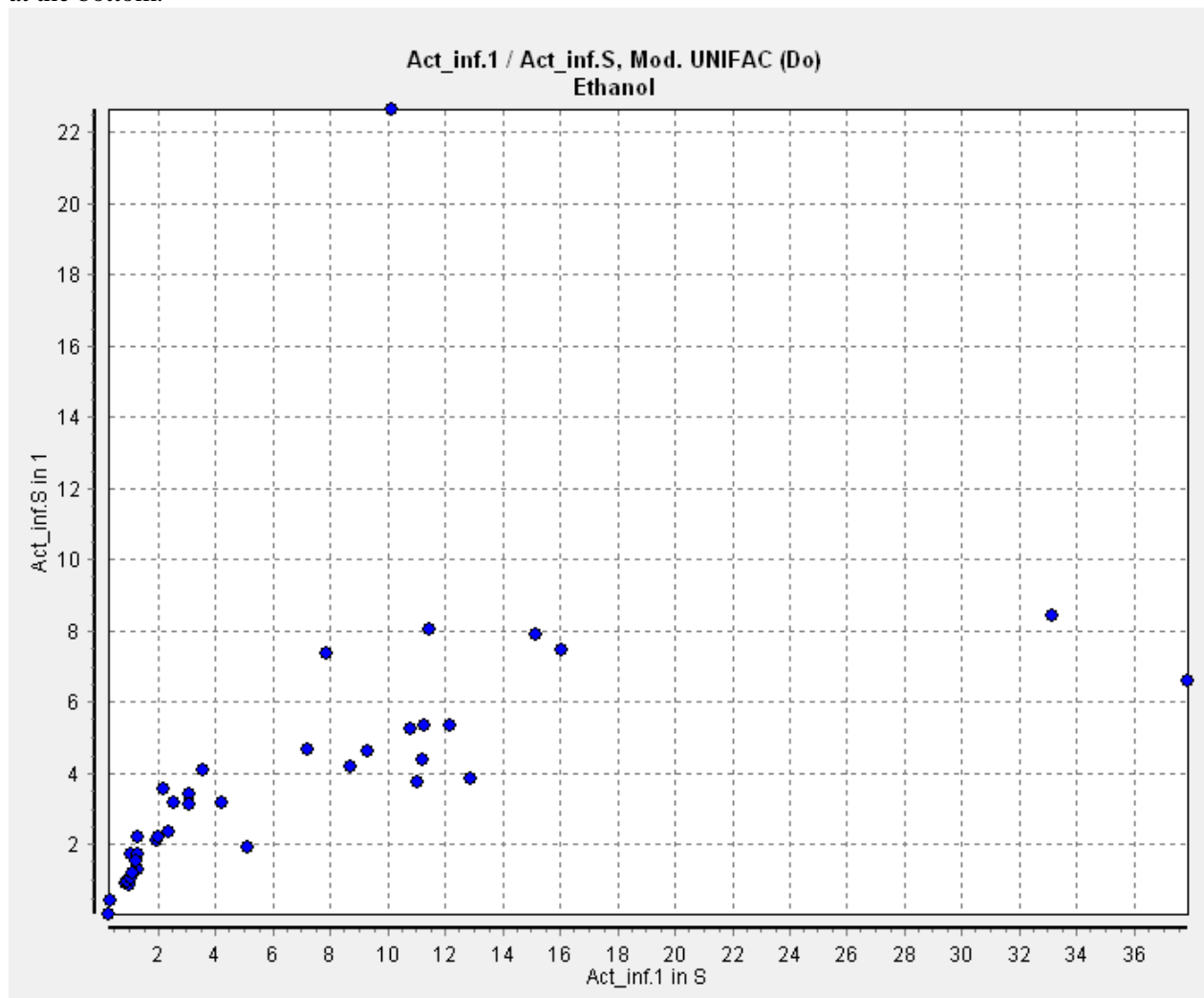
Numbers mark the given components. S marks the tested component

DDB Nr.	T [K]	Act 1 in S	Act S in 1	Psat 1 [kPa]	Psat S [kPa]	Psat 1/Psat S	AZD 1 S
1	323.00	0.932942	0.963623	29.2128	263.326	0.110938	None Acetaldehyde
2	323.00	0.889133	0.883587	n.a.	n.a.	n.a.	n.a. Acetamide
3	323.00	3.10404	3.4345	29.2128	33.8765	0.862331	Positive Acetonitrile
4	323.00	1.95287	2.09795	29.2128	80.9605	0.360827	None Acetone
5	323.00	0.278885	0.0399946	29.2128	6.53607	4.46947	None Ethylenediamine
6	323.00	7.21078	4.66812	29.2128	5.56908	5.24553	None 1,2-Dibromoethane
7	323.00	11.0551	3.74572	29.2128	148.306	0.196976	Positive Ethyl bromide
8	323.00	1.31162	1.31277	29.2128	0.11356	257.244	None 1,2-Ethandiol
9	323.00	12.1836	5.31729	29.2128	47.4049	0.61624	Positive Ethyl iodide
10	323.00	1.29166	2.22234	n.a.	n.a.	n.a.	n.a. 5-Ethyl-2-nonanol
12	323.00	4.22292	3.15011	29.2128	170.142	0.171696	None Diethyl ether
13	323.00	0.999729	0.879719	29.2128	385.619	0.0757555	None Ethylene oxide
14	323.00	1.06127	1.0864	29.2128	13.3541	2.18754	None 2-Propen-1-ol
16	323.00	3.06495	3.14298	29.2128	87.4146	0.334186	Positive Formic acid ethyl ester
17	323.00	2.53841	3.15101	29.2128	0.435075	67.1442	None Aniline
18	323.00	3.53589	4.06319	n.a.	n.a.	n.a.	n.a. Anisole
19	323.00	1.06865	1.70422	29.2128	5.57863	5.23655	None 2-Picoline
20	323.00	16.0316	7.44499	29.2128	2.33645	12.503	None .alpha.-Pinene
21	323.00	2.35463	2.37148	29.2128	37.7465	0.77392	Positive Ethyl acetate
22	323.00	1.08289	1.12209	29.2128	10.7651	2.71366	None 2-Butanol

The table uses the following abbreviations

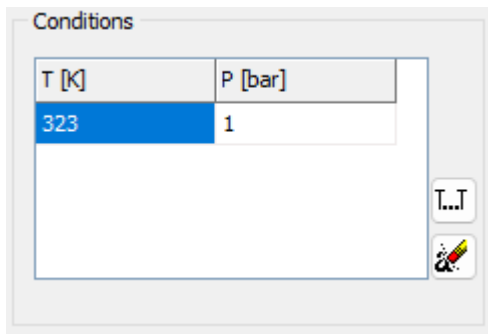
Column	Description
T	Temperature
Act 1 in S	Activity Coefficient of component 1 at infinite dilution in the solvent
Act S in 1	Activity Coefficient of the solvent in infinite dilution in component 1
Psat 1	Vapor pressure of component 1
AZD 1 S	Azeotropic behavior in the system component 1 with the solvent (explanation see chapter Act_inf)
n.a.	Vapor pressure is missing

Activity coefficient pairs are displayed in a diagram. The solvent information of every point is with its values at the bottom.



3.4 Excess properties

All excess properties have very similar calculation options. Under “Conditions” it is possible to define calculation temperatures and calculation pressures for models with an equation of state.



At the bottom, the concentrations can be defined for the calculation. The handling is very similar to the VLE options.

3.4.1 HE

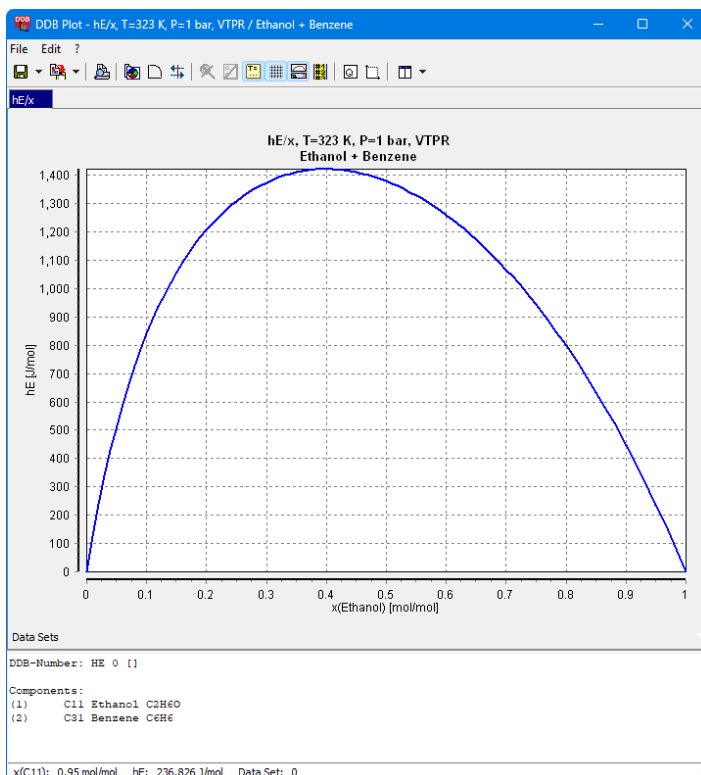
This property calculates the excess enthalpies for a given system. This calculation is possible with all models. However, the pressure is only used for models with an equation of state.

Result

The results are shown after the component and parameter list.

T [K]	P [bar]	hE [J/mol]	x1	x2
323.00	1.00	0.00	0.00000	1.00000
323.00	1.00	125.13	0.01000	0.99000
323.00	1.00	237.54	0.02000	0.98000
323.00	1.00	339.03	0.03000	0.97000
323.00	1.00	431.08	0.04000	0.96000

T is for temperature, P is for pressure and hE for excess enthalpy. For each component, the liquid concentration is given as x. The results are additionally shown as diagram.



This diagram can be printed, saved or copied. It is also possible to edit the chart.

3.4.2 VE

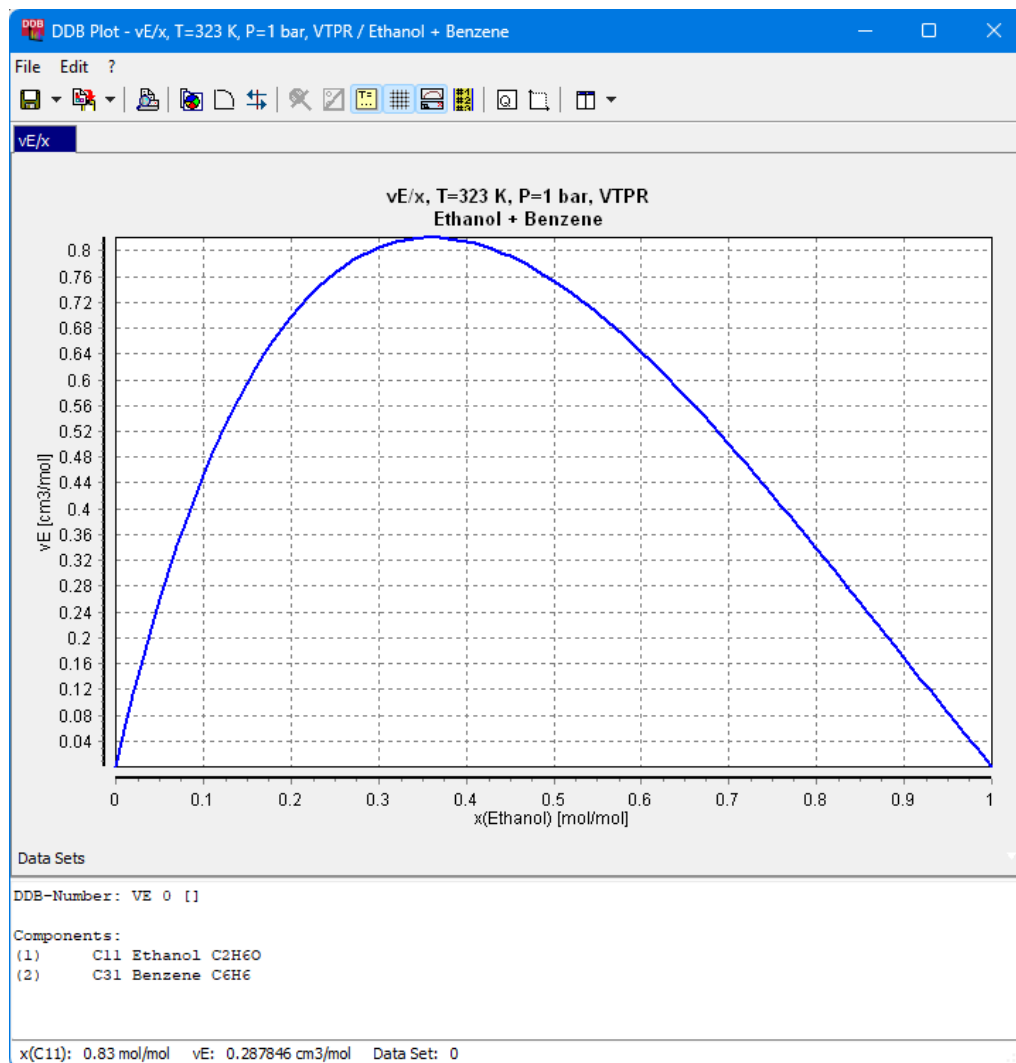
Excess volumes can only be calculated by models with an equation of state.

Result

The results are shown after the component and parameter list.

T [K]	P [bar]	vE [cm ³ /mol]	x1	x2
323.00	1.00	0.0000	0.00000	1.00000
323.00	1.00	0.0577	0.01000	0.99000
323.00	1.00	0.1121	0.02000	0.98000
323.00	1.00	0.1635	0.03000	0.97000
323.00	1.00	0.2120	0.04000	0.96000

T is for temperature, P is for pressure and vE for excess volume. For each component, the liquid concentration is given as x. The results are additionally shown as diagram.



This diagram can be printed, saved or copied. It is also possible to edit the chart.

3.4.3 CPE

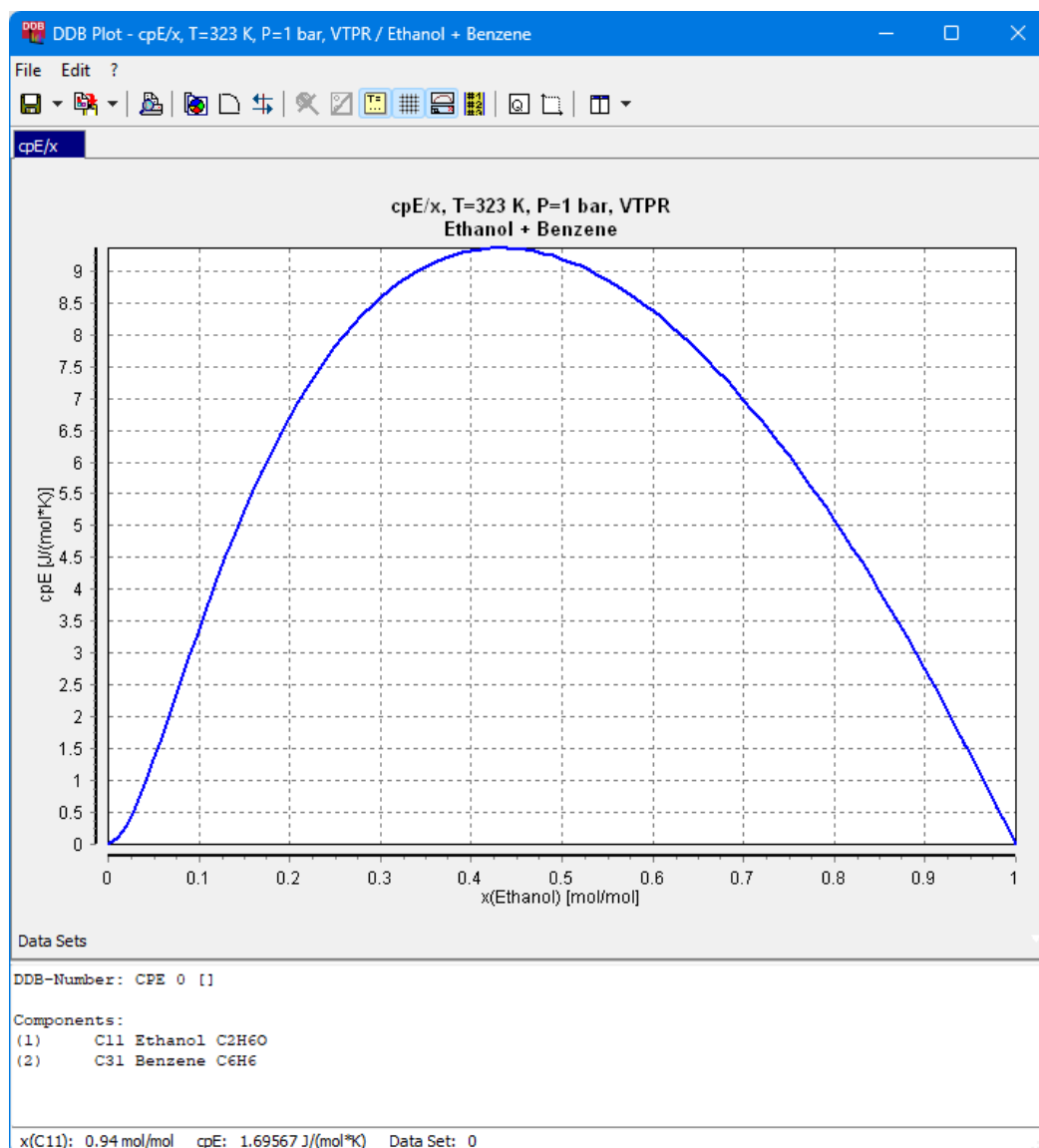
This property calculates the excess heat capacities for a given system. This calculation is possible with all models. However, the pressure is only used for models with an equation of state.

Result

The results are shown after the component and parameter list.

T [K]	P [bar]	cpE [J/mol/K]	x1	x2
323.00	1.00	0.0000	0.00000	1.00000
323.00	1.00	0.0883	0.01000	0.99000
323.00	1.00	0.2982	0.02000	0.98000
323.00	1.00	0.5912	0.03000	0.97000
323.00	1.00	0.9396	0.04000	0.96000

T is for temperature, P is for pressure and cpE for excess heat capacity. For each component, the liquid concentration is given as x. The results are additionally shown as diagram.



This diagram can be printed, saved or copied. It is also possible to edit the chart.