DDBST
Dortmund Data Bank
Software & Separation
Technology

Predict

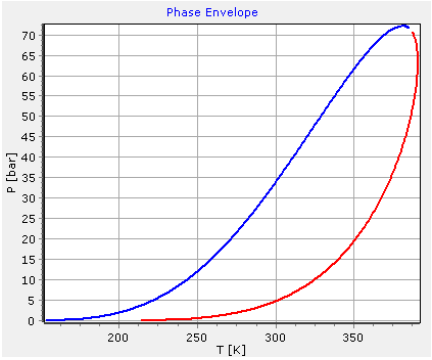
Calculation of Vapor-Liquid Equilibria, Solubilities, Activities and Excess Properties with the Models PSRK, VTPR, UNIFAC, Mod. UNIFAC, NIST-mod. UNIFAC(Do), mod. UNIFAC(Ly) and a Variety of EOS Mixing Rules.

Description

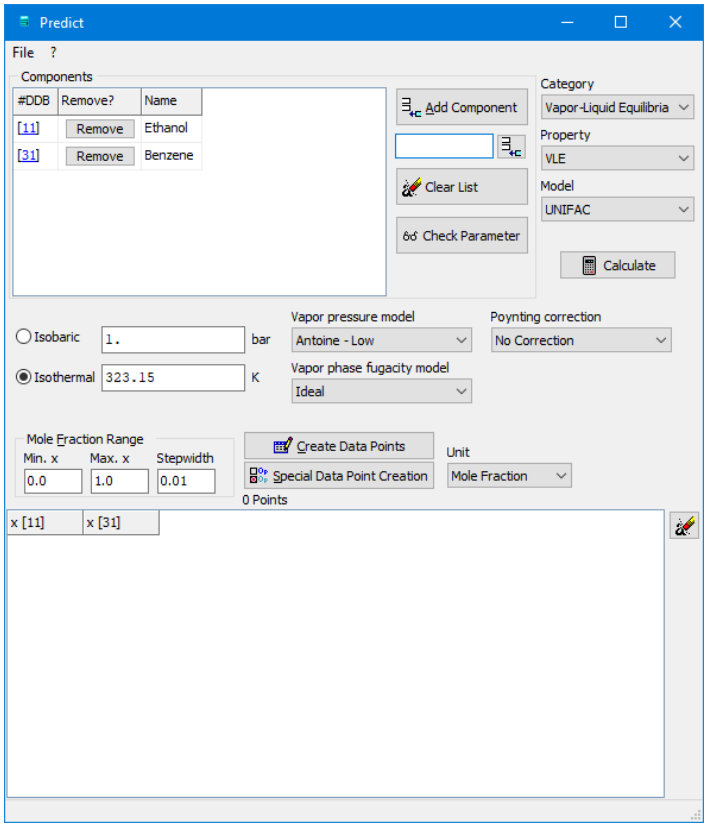
The stand-alone package Predict allows a multitude of multicomponent mixture calculations using the thermodynamic models Predictive Soave-Redlich-Kwong (PSRK) and Volume-Translated-Peng-Robinson (VTPR) equations of state and the group contribution methods UNIFAC, Mod. UNIFAC(Do), NIST-mod. UNIFAC and Mod. UNIFAC (Ly). Calculations with EOS mixing rules are also possible. The supported calculations are:

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

Results are displayed in tables and diagrams and can be copied to the Windows clipboard, saved to file or printed.



Phase Envelope Calculation with VTPR: Carbon dioxide and *n*-Butane



Main Menu

Applications

The methods and calculations are used in a large variety of applications also including risk assessment to calculate the maximum pressure in a vessel after overheating of a reaction system.

Scope of Supply

The software comes with

- the latest published parameter matrices for all the estimation methods PSRK, VTPR, UNIFAC, Mod. UNIFAC(Do), NIST-mod. UNIFAC and Mod. UNIFAC (Ly).
- structural group lists for all possible components

Members of the UNIFAC-Consortium (www.unifac.org) have access to the latest PSRK, VTPR. UNIFAC and Mod. UNIFAC parameters.

Changes and errors are possible regarding all information.