CHAPTER VIII
STRUCTURE AND USING THE PROGRAM

This chapter presented produce of development of a database programming for searching and estimating properties of gases and liquids and the methods for using the program. Linking this program with the other programs is also included in this chapter.

8.1 THERMODYNAMIC MODEL

In this work, Redlich-Kwong(RK), Soave-Redlich-Kwong(SRK), and Peng-Robinson(PR) equations are used to predict thermodynamic properties of gases and liquids. For Vapor-liquid equilibria, Raoult's law is introduced to predict the properties of gas and liquids for ideal solutions. SRK and PR equations are used to predict these properties of nonideal solutions.

8.2 ASSUMPTIONS AND RESTRICTIONS OF THE PROGRAM

8.2.1 Assumptions

The assumptions for estimating properties of gases and liquids are as follows:

- Neglected heat of mixing between the mixtures.
- Neglected binary interaction parameters therefore, $k_{ij} = 0$.
- Reference state for calculating enthalpy and entropy changes is at ideal gas state, temperature at 273.15 K and pressure at the system pressure.

8.2.2 Limitation

This program can be used for

- Normal fluid (nitrogen, oxygen, carbonmonoxide, and hydrocarbons).
- Nonpolar substances and slightly polar substances.
- Subcritical region.

This program can not be used for

- Polar compounds.
- Large molecules (polymers) and electrolytes
- Estimation fugacity and fugacity coefficient of liquid mixture.

8.3 STRUCTURE AND LINKING WITH THE OTHER PROGRAMS

A database program for searching and estimating properties of gases and liquids is composed of six main parts as follows:

1. Database for collecting thermodynamic properties and transport properties. One part stores thermodynamic properties such as critical temperature, critical pressure, critical volume, critical compressibility factor. The other part stores transport parameters, which are constants for calculating liquid viscosity. Data in the database will be stored in form of text file.

2. Database management system for accessing data in the database and transfering data to other programs.

3. Searching properties of a compound is used to search the physical and thermodynamic properties of gas and liquid in a database.

4. Estimation thermodynamic properties is used to predicting thermodynamic properties of gases and liquids together with vapor-liquid equilibria.

5. Interface on Windows is used to show the results of prediction thermodynamic properties, transport property and the properties of a compound.

6. Linking with the other programs is written in the same language (Turbo C^{++}). This program has been designed with main program for linking to other programs by transfering data from the main program to other programs. This program is written with the concept of object -oriented programming(OOP) .

Figure 8.1 shows a structure of the program and method for linking with the other programs which must be written in the same language.

8.4 COMPOSITION OF THE MAIN PROGRAM

When the program is executed, the first menu is appeared as Figure 8.2. The menu is composed of File, Select, Estimate, Run and Help command.

8.4.1 File commamd

File command consists of exit command which is used for exit the program and return to main menu of Windows as shown in Figure 8.3.

8.4.2 Select command

Select command consists of Single component command, Multicomponent command, and Viscosity component command as shown in Figure 8.4.

Single component command is used for selecting a compound for searching properties and estimating vapor pressure, heat of vaporization, as shown in Figure 8.5.

Multicomponent command is used for seclecting compounds for estimating compressibility factor, molar volume, fugacity, fugacity coefficient, enthalpy, entropy, enthalpy and entropy departure, vapor-liquid equilibria (bubble-point pressure, dew-point pressure, bubble-point temperature, dew-point temperature, and isothermal flash) as shown in Figure 8.6.

Viscosity command is used for selecting a compound for estimating liquid viscosity as shown in Figure 8.7.

8.4.3 Estimate command

Estimate command is used for estimating thermodynamic properties, transport property, and vapor-liquid equilibria. Figure 8.8 shows Estimate command and Figure 8.9 is an example for estimating bubble-point pressure. User must input temperature and mole fractions for calculating bubble-point pressure.

8.4.4 Run command

Run command consists of Search command and Result command . Search command is used for showing the results of searching the properties of gas and liquid. Result command shows the results of estimating properties of gases and liquid. Run command is shown in Figure 8.10

8.4.5 Help command

Help command has the detail about the methods for using keyboard when there is no mouse on a personel computer . Help command is shown in Figure 8.11.

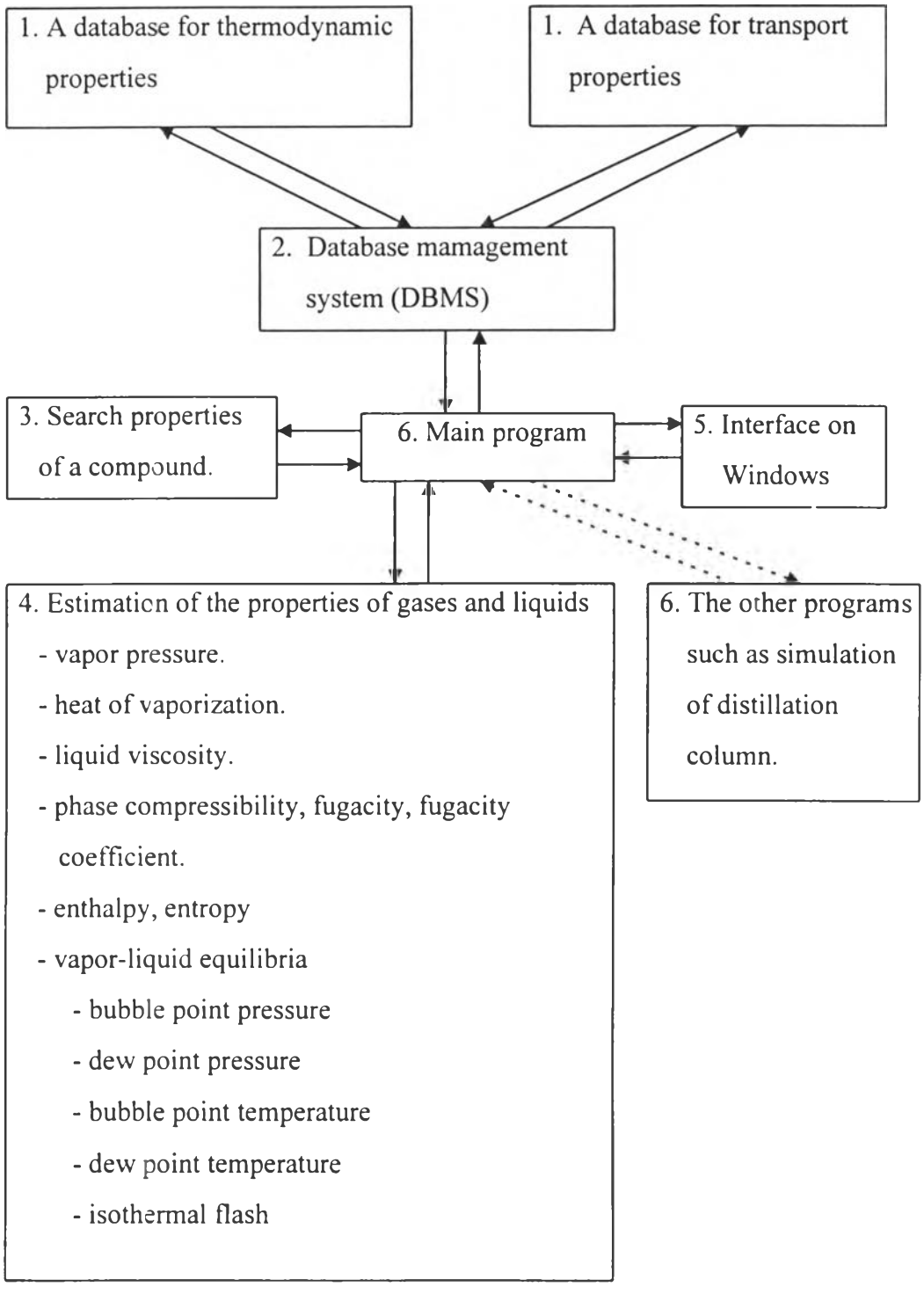

Figure 8.1 Structure of a database system for searching and estimating properties of gases and liquids

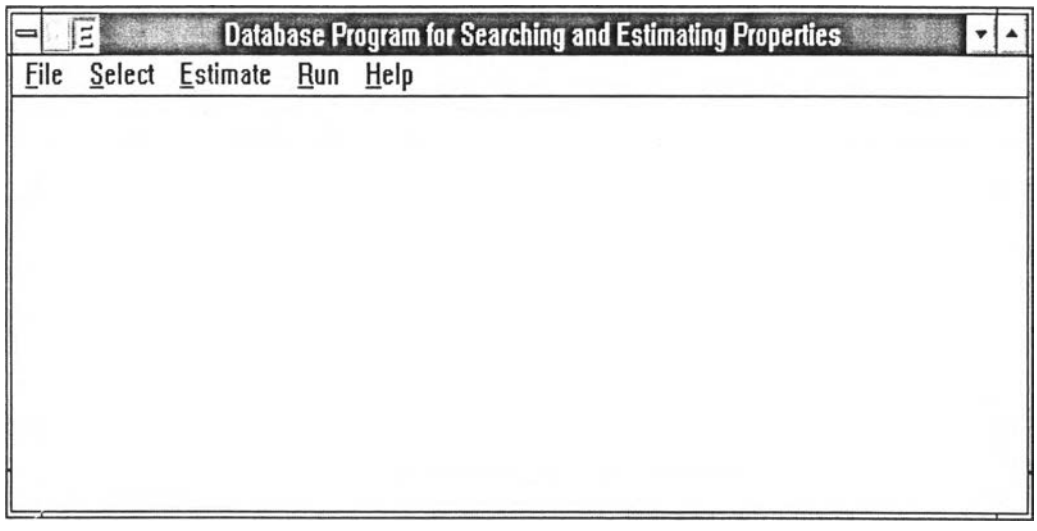

Figure 8.2 Menu of a database program for searching and estimating properties of gases and liquids

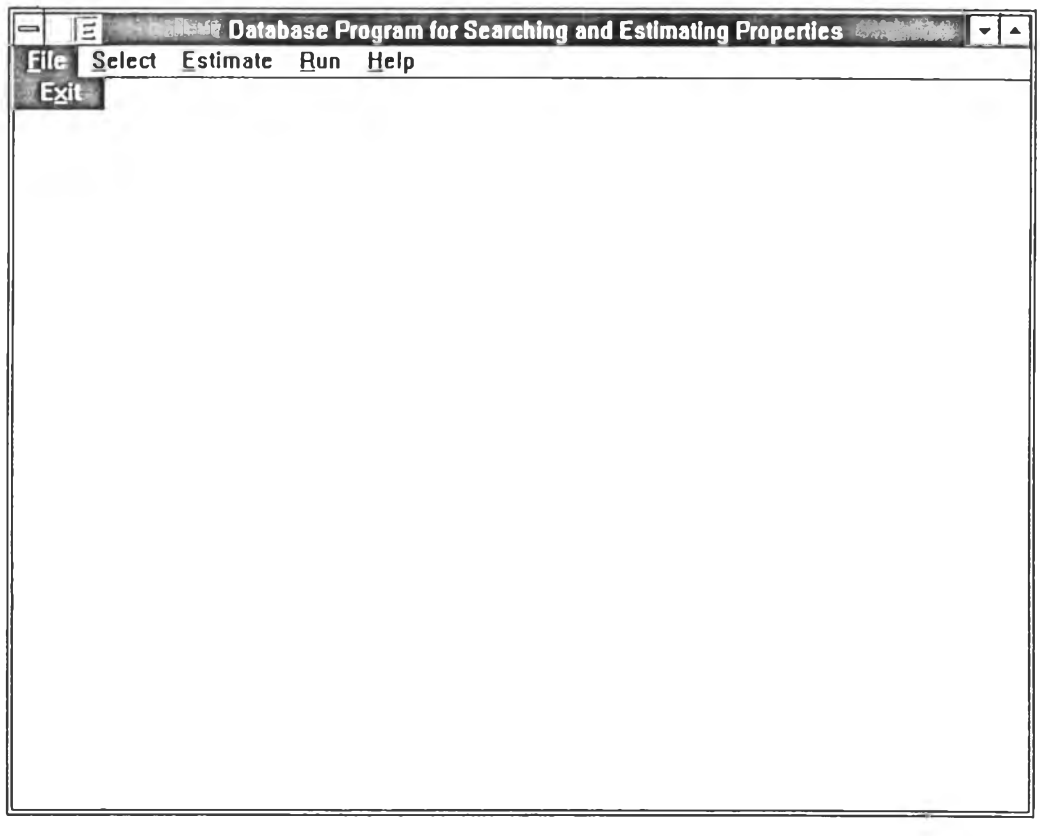

Figure 8.3 Menu of File command

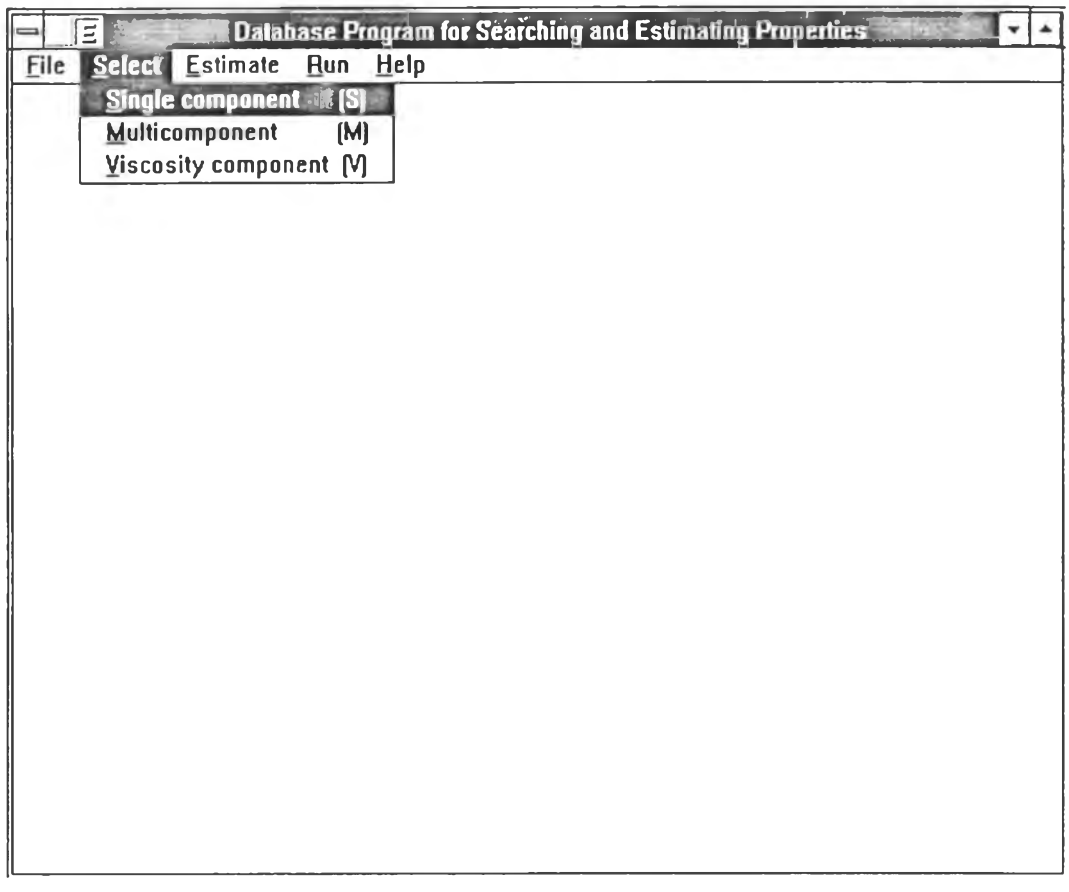

Figure 8.4 Menu of Select command

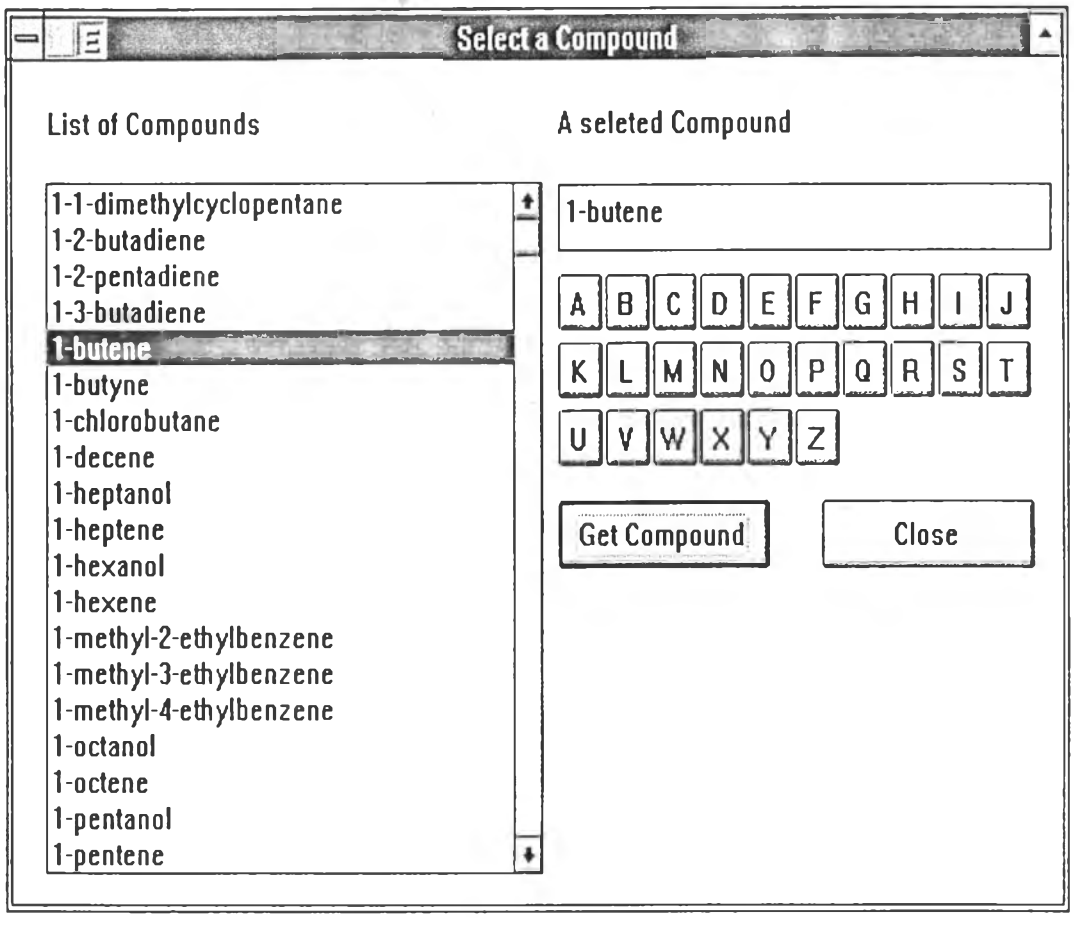

Figure 8.5 Windows of Single component command

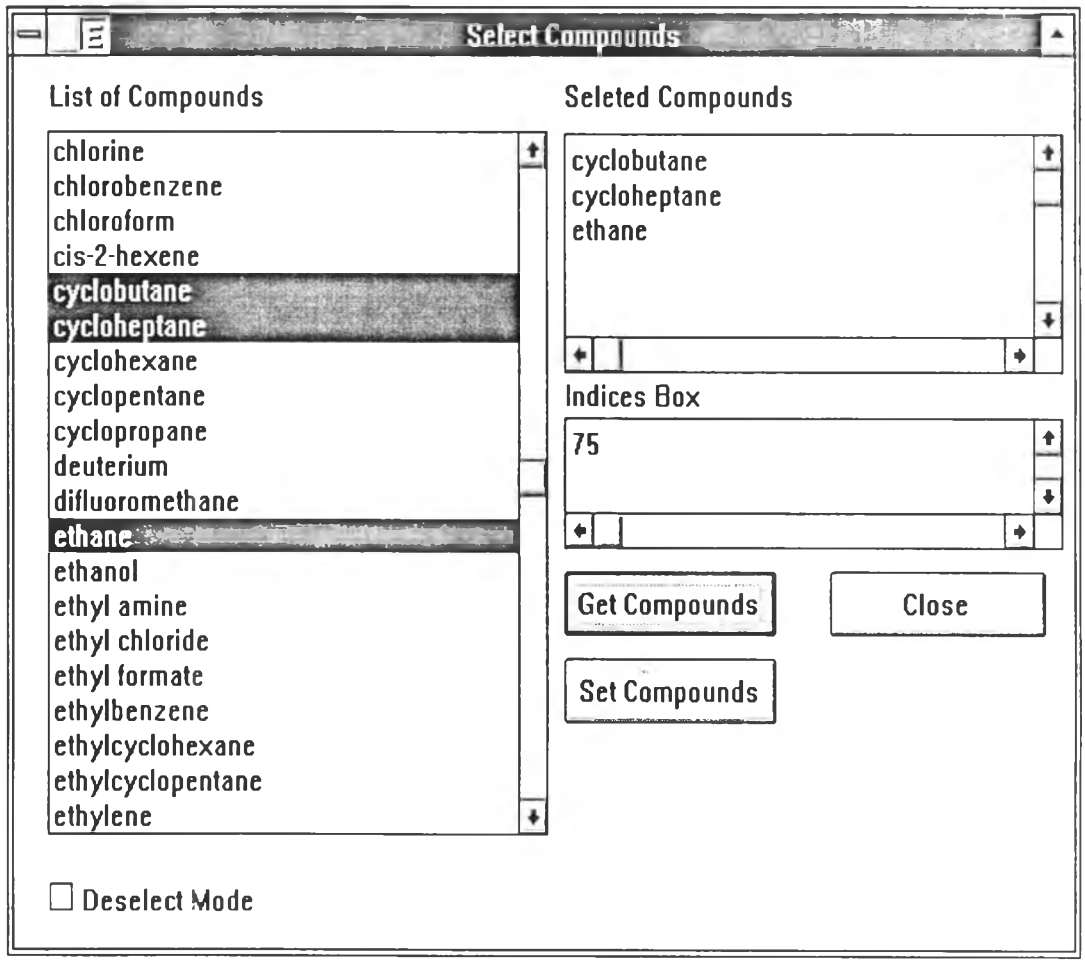

Figure 8.6 Windows of Multicomponent command

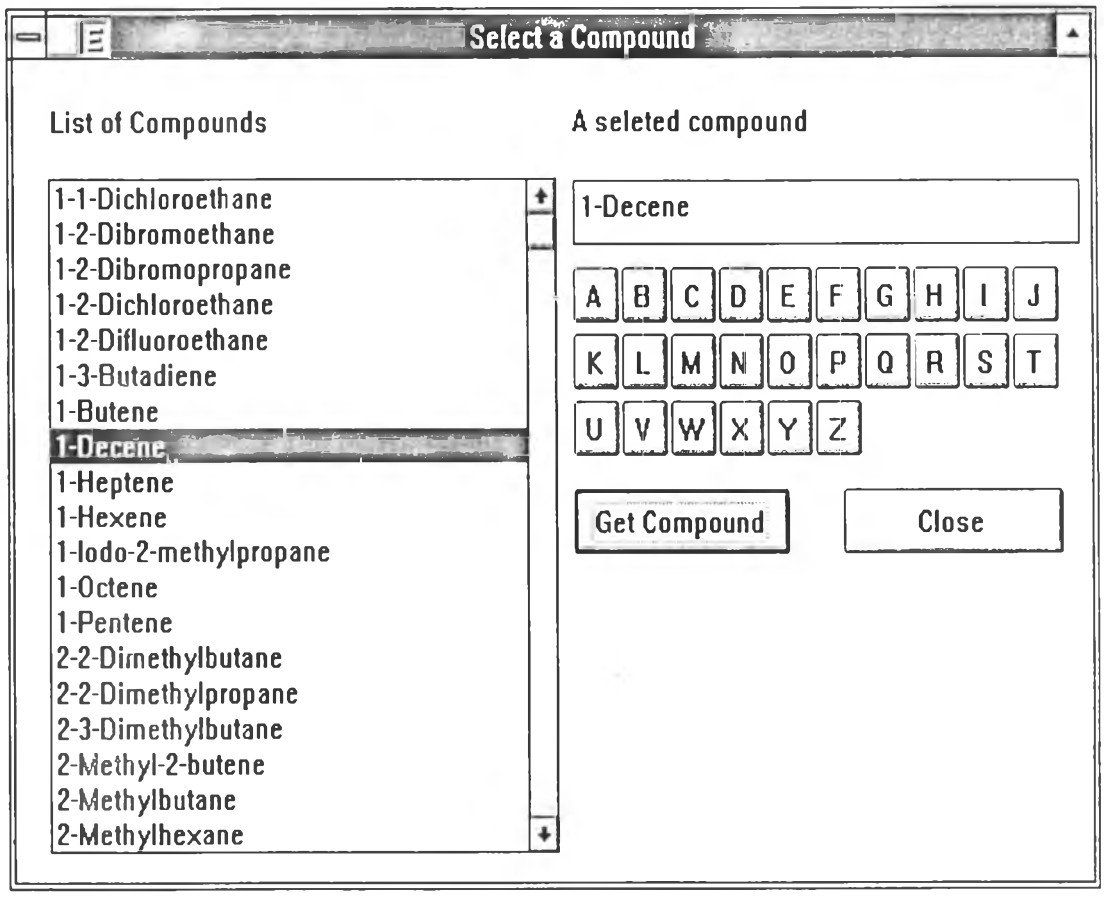

Figure 8.7 Windows of Viscosity command

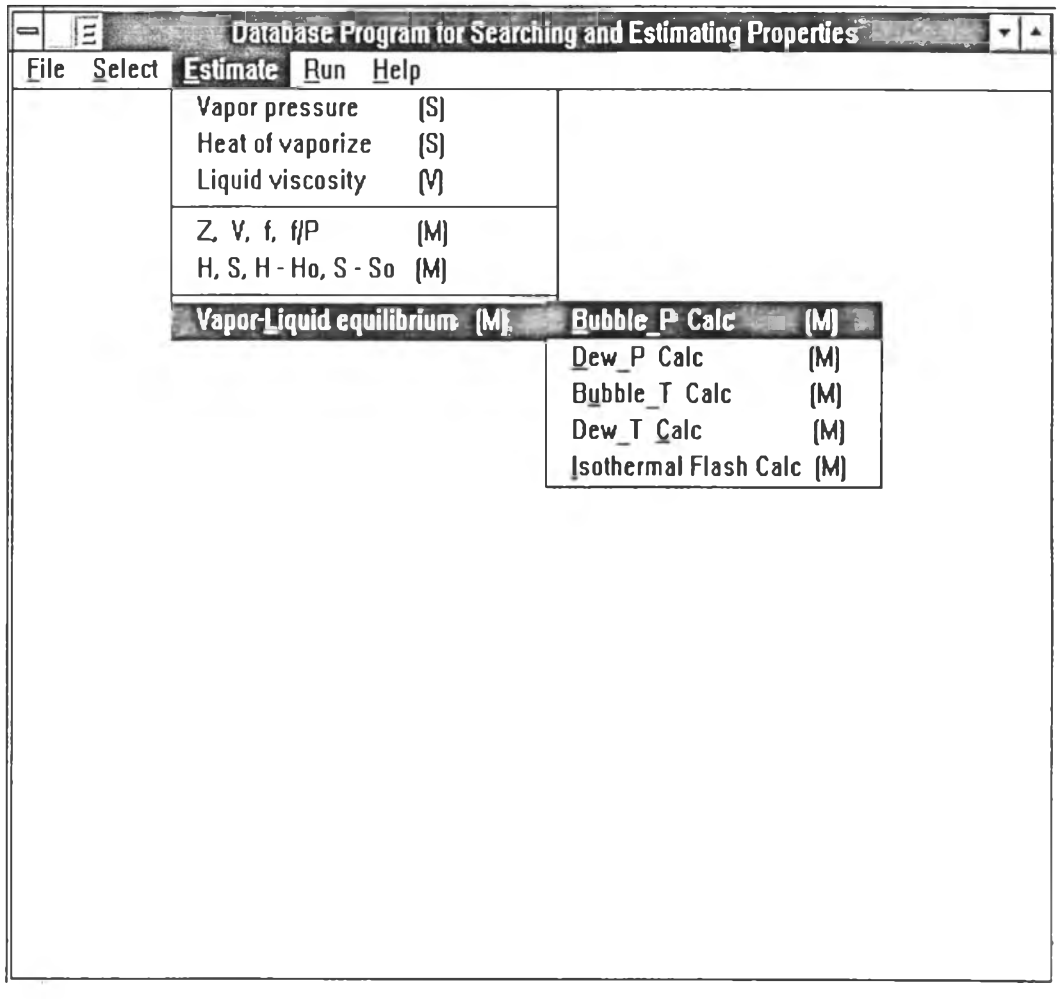

Figure 8.8 Menu of Estimate command

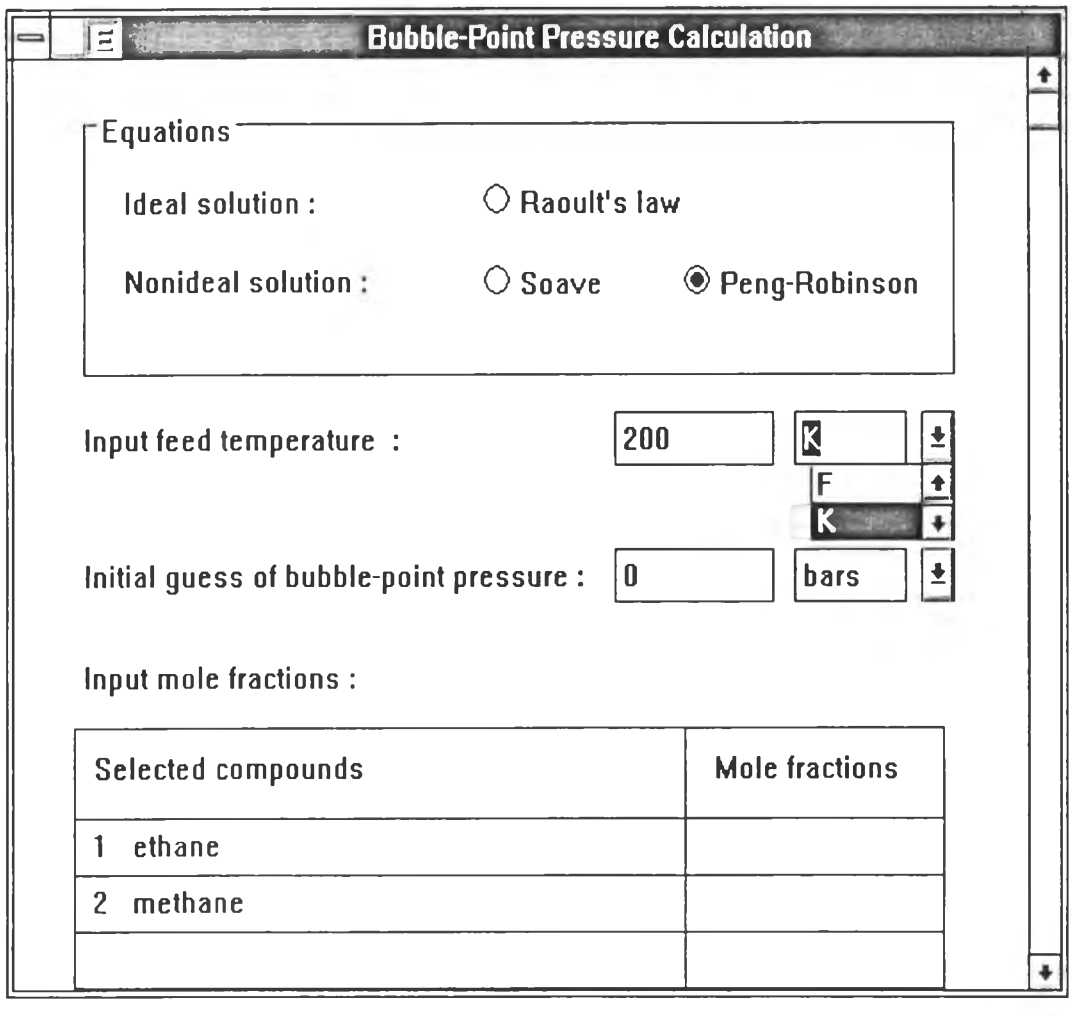

Figure 8.9 Windows of bubble-point pressure calculation

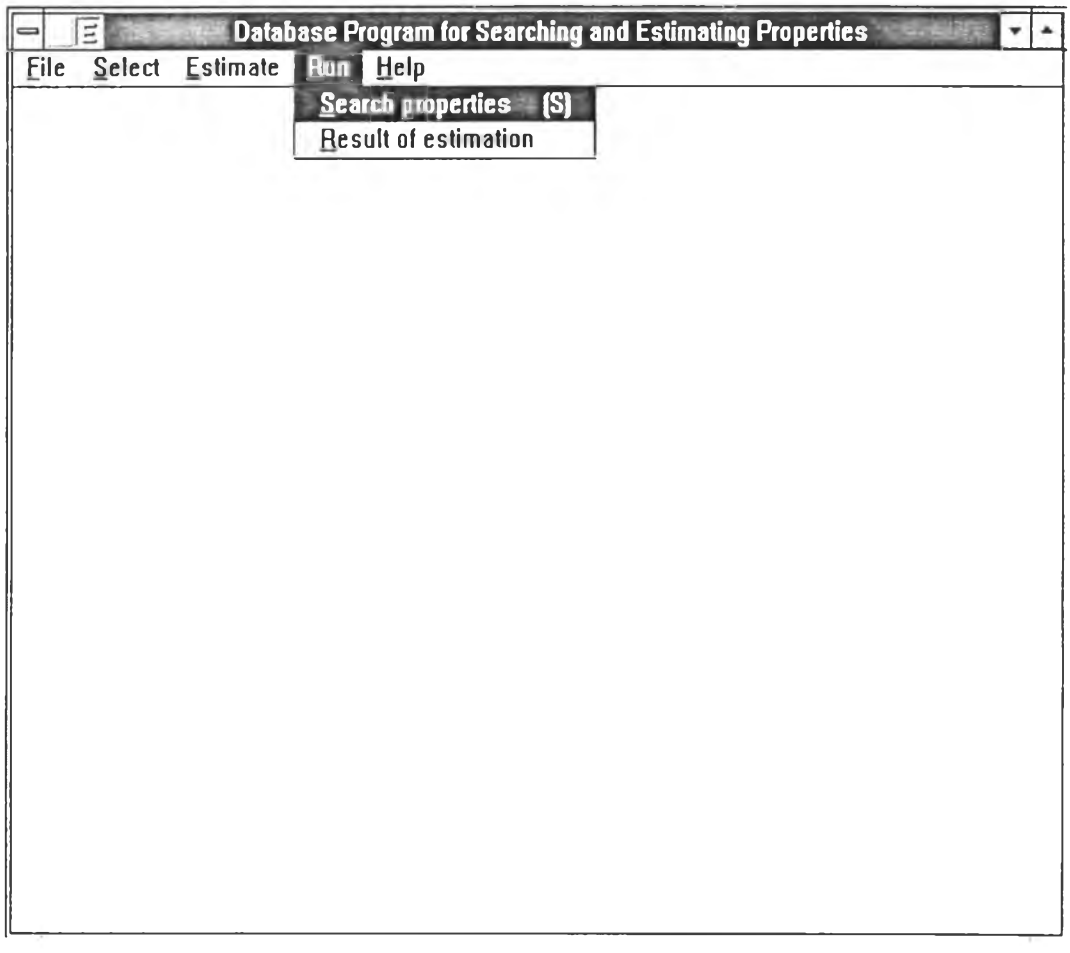

Figure 8.10 Menu of Run command

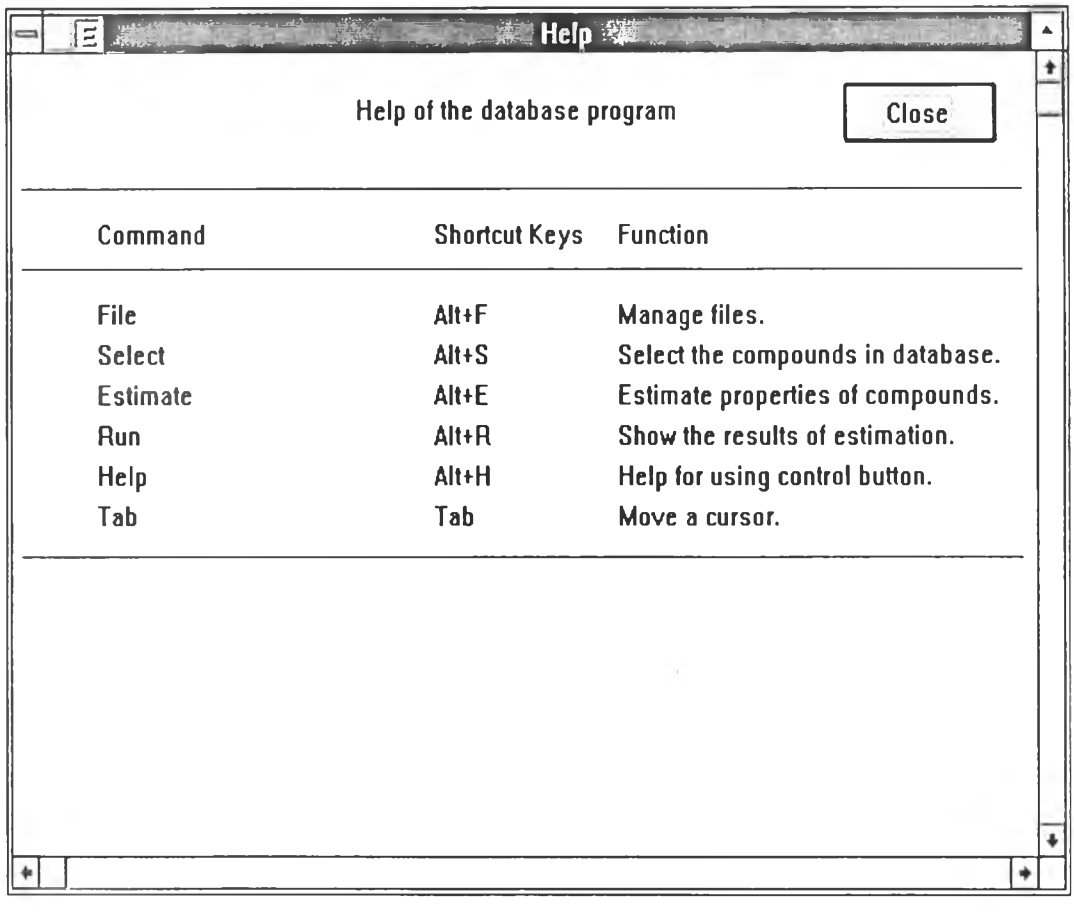

Figure 8.11 Windows of Help command.