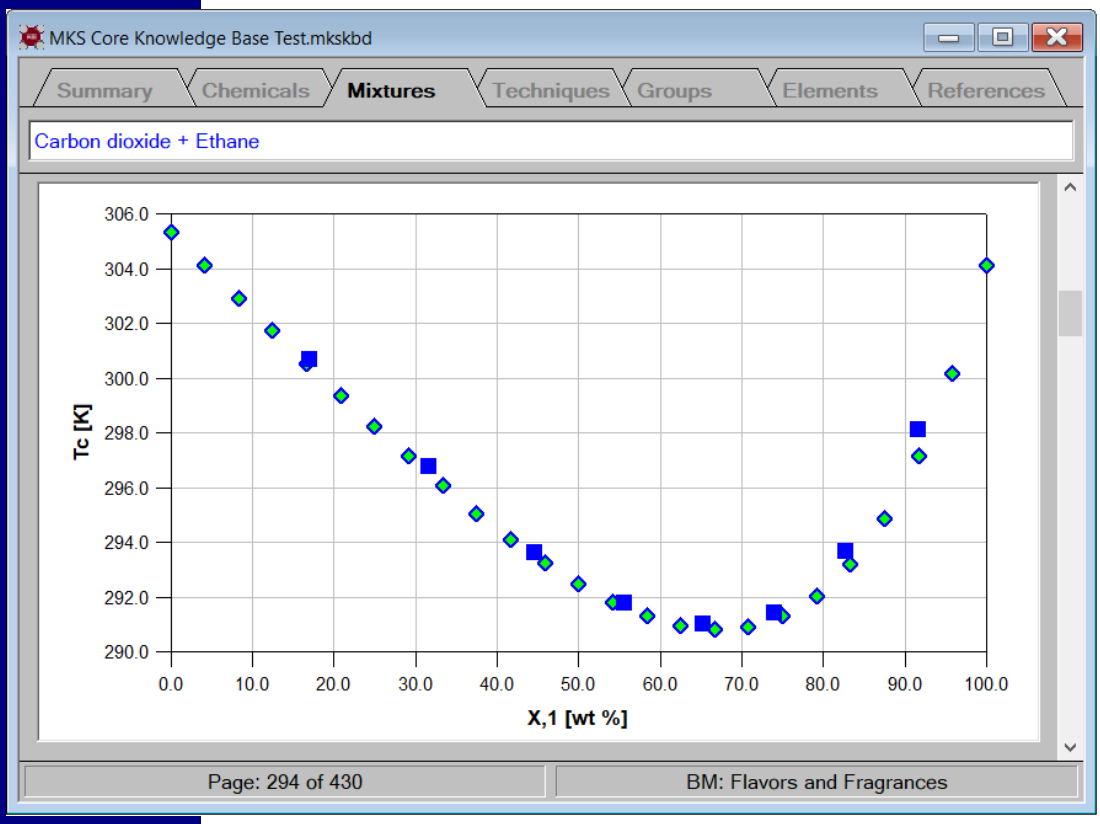
CRANIUM®

FAST, ACCURATE, AND EASY PHYSICAL PROPERTY ESTIMATION

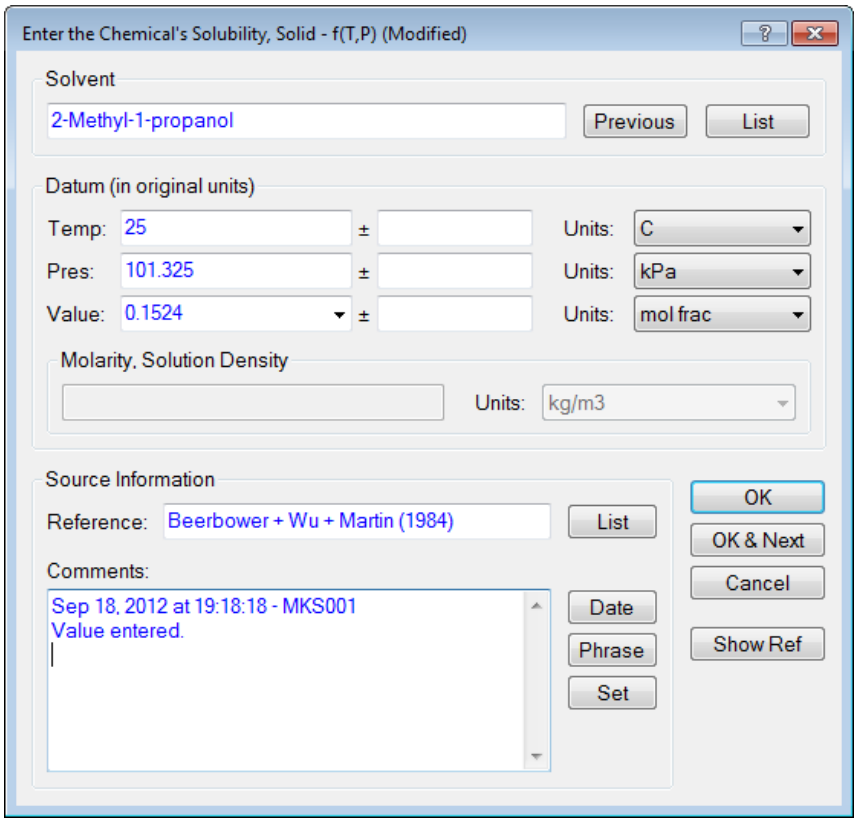


Easily calculate property estimates for chemicals and mixtures.

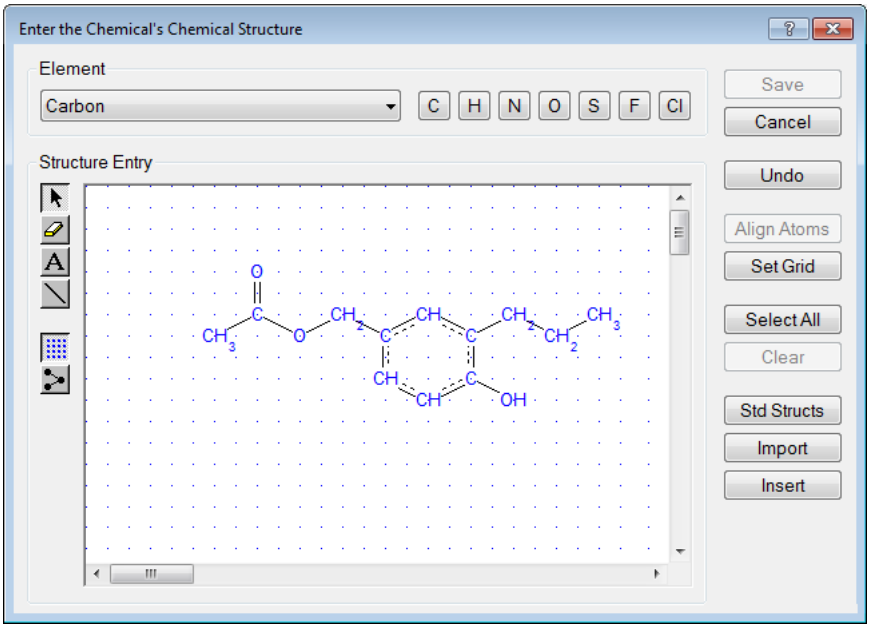
Physical property values are essential for designing, simulating, and optimizing chemical processes and products. Invariably, for the particular chemicals, compositions, temperatures, and pressures you are working with, data is not available. Fortunately, there is a computer software program which provides accurate estimates for many physical properties.

Cranium is an advanced physical property estimation system capable of predicting values for more than 40 physical properties. Estimates are generated for both chemicals and mixtures. Simply draw your compound's molecular structure or enter its composition and Cranium will automatically analyze the structure for important functional groups, select the best estimation technique, retrieve any required property data, and provide you with the most accurate estimate possible.

Cranium stores data on elements, molecular structures, pure chemicals, mixtures, and physical property estimation techniques in knowledge bases. MKS distributes knowledge bases covering common chemicals, hydrocarbons, refrigerants, solvents, fragrances and many more. You may find these databases sufficient for most of your physical property data needs. However, Cranium's capabilities go far beyond a simple database program.



You can quickly and easily enter data using specialized dialog windows. Cranium checks your entries for completeness and accuracy.



Estimate a chemical's properties by simply drawing its structure using Cranium's molecular editor.

INTUITIVE USER INTERFACE

Cranium's user interface is designed around the theme of an electronic reference book. Tabbed "chapters" organize information on elements, structural groups, chemicals, mixtures, estimation techniques, and references. Each chapter further organizes information into individual pages. Each "page" displays data on a single database entry, e.g., a chemical or mixture. This analogy to printed reference books makes Cranium very easy to use.

You enter new data into Cranium using tailored dialog windows. Each dialog provides buttons and lists which assist you in data entry. Before the data is stored the dialog checks for completeness and accuracy.

MOLECULAR STRUCTURE MANAGEMENT

Identifying group fragments in a molecular structure is one of the most tedious and error prone steps of using estimation techniques. This is complicated by the fact that invariably each technique uses its own unique combination of groups. Cranium eliminates this tedious step by providing a graphical structure editing interface which records all the connectivity information needed to automatically dissect a structure into groups. All you need to do is draw the molecule's structure.

IMPORT & EXPORT STRUCTURES AND DATA

You can use Cranium as a central repository of your physical property values. Data and estimates can be copied and pasted between Cranium and word processors or spreadsheets. Cranium's file export capability enables you to generate input files for other process simulation and design software. Cranium can import molecular structures directly from MOL or SD files.

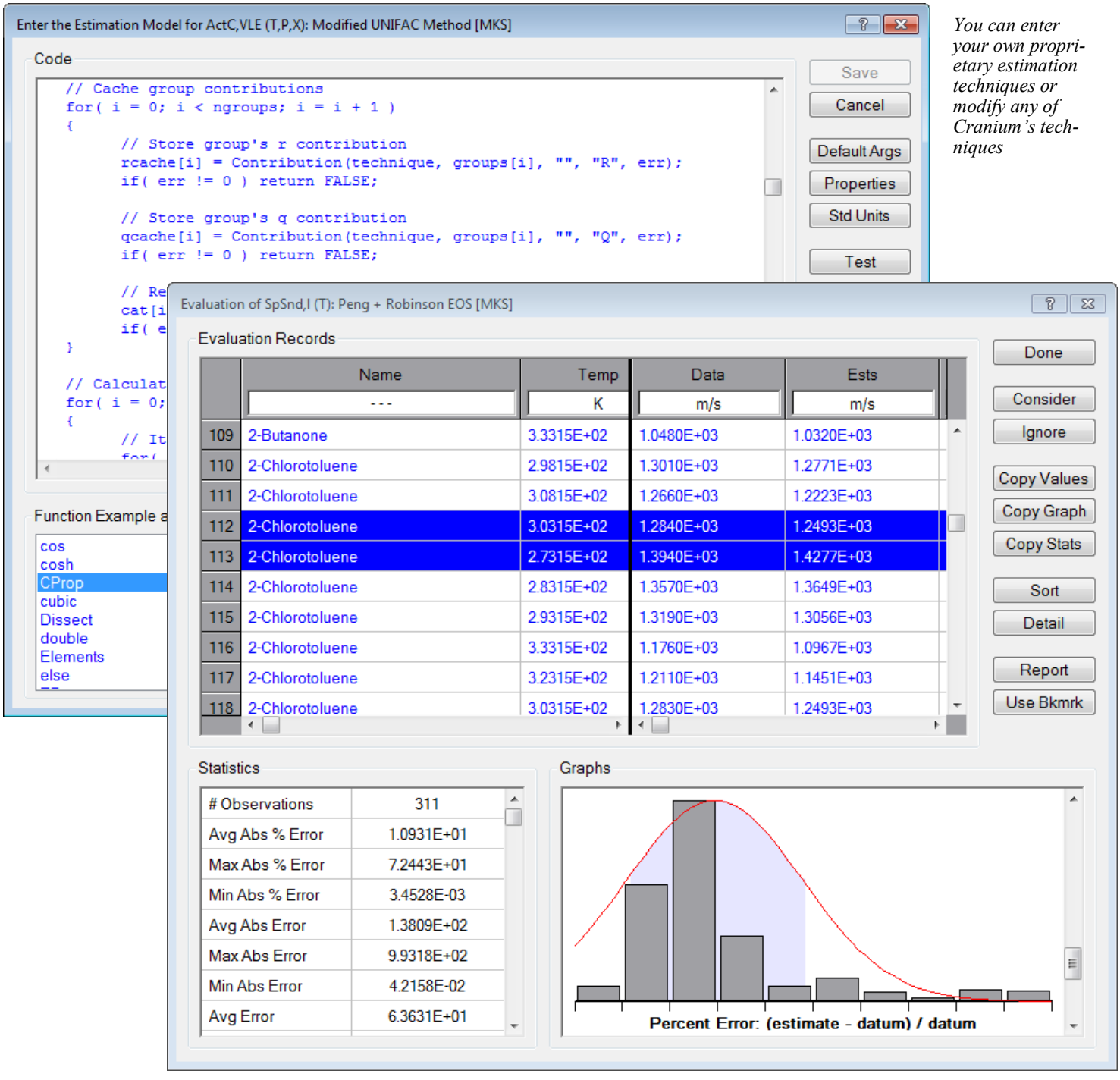
Cranium also gives you the ability to create your own, proprietary databases for royalty-free distribution to other Cranium users. Simply enter data and estimation techniques on your specific compounds or copy them from other Cranium databases.

POWERFUL ESTIMATION ENGINE

When you ask Cranium to estimate a chemical's properties it begins by collecting all applicable estimation techniques. Cranium then analyzes these techniques finding the one which is most appropriate for your entered compound. If Cranium requires other properties to perform the estimation it automatically searches for available data and, if no data are found, repeats the previous steps to estimate the required property.

The ability to enter your own estimation techniques is one of Cranium's most powerful features. Using a C-like language you can enter your estimation code directly into Cranium. A set of library routines give you access to mathematical functions, structural analysis functions, and property estimation techniques. Cranium compiles your entered code into a fast, executable function. You can enter most estimation techniques in only a few minutes.

Typically published estimation techniques are developed for a broad range of chemicals. Tailoring these techniques to focus on only those chemicals of interest to you can dramatically improve estimation accuracy. Once you enter your new estimation techniques, Cranium can automatically evaluate them by comparing their estimates against stored experimental data. An error analysis will quickly tell you if the new technique is appropriate for your compounds of interest.



You can enter your own proprietary estimation techniques or modify any of Cranium's techniques

KEY CAPABILITIES

- Automatically estimate over 40 physical properties
- Estimate a pure component's properties by simply drawing its molecular structure
- Estimate a mixture's properties by simply entering its components and composition
- Import molecular structures from popular data formats
- Document source and comments about each physical property data point.
- Enter your own proprietary data and tailored estimation techniques
- Create, compile and distribute your own physical property databases
- Copy and paste physical properties into your favorite Windows programs
- Organize your company's property data in one place
- Export property estimates to simulation programs

PROPERTIES ESTIMATED

- Absolute Entropy
- Acentric Factor
- Activity Coefficient
- Aquatic Toxicity
- Autoignition Temperature
- Bioconcentration Factor
- Biological Oxygen Demand
- Boiling Point
- Chemical Oxygen Demand
- Critical Pressure
- Critical Temperature
- Critical Volume
- Densities
- Diffusion Coefficient
- Enthalpy of Formation
- Enthalpy of Fusion
- Enthalpy of Vaporization
- Flammability Limits
- Flash Point
- Freezing Point
- Fugacity Coefficient
- Gibbs Energy of Formation
- Heat Capacities
- Henry's Law Constant
- Liquid-Liquid Equilibria
- Melting Point
- Molecular Weight
- Octanol-Water Partition
- Refractive Index
- SLE Liquidus Point
- Solubility Parameter
- Speed of Sound
- Surface Tension
- Thermal Conductivities
- Vapor Pressures
- Vapor-Liquid Equilibria
- Viscosities
- VLE Bubble Point
- VLE Dew Point
- Water Solubility

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