

# CRANIUM™

FAST,  
ACCURATE,  
AND EASY  
PHYSICAL  
PROPERTY  
ESTIMATION

The screenshot shows the Organics.crn software window. The title bar reads "Organics.crn". The menu bar includes "Intro", "Elements", "Groups", "Materials", "Mixtures", "Techniques", and "References". The main window title is "Ethylene + Methylamine". Below this, the section "Constant Properties:" is displayed. A "Property:" field contains "Critical Temperature". A table below shows data for five components (A, B, C) with their respective weight percentages and estimated critical temperatures. The table has columns for "A wt %", "B wt %", "C wt %", "Data K", and "Ests K". The data rows are numbered 1 through 5. At the bottom of the window, there are "Prev", "Compute", and "Next" buttons, and a page indicator "Page 27 of 70".

	A wt %	B wt %	C wt %	Data K	Ests K
1	84.623	15.377	---	304.700	301.880
2	74.412	25.588	---	323.400	315.427
3	70.844	29.156	---	327.600	320.274
4	63.785	36.215	---	336.500	330.043
5	55.099	44.901	---	350.600	342.402

*Easily calculate property estimates for pure components and mixtures.*

Physical property values are essential for process design, simulation, and optimization. Invariably, for the particular compounds, 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 20 physical properties. Estimates are generated for both pure components and mixtures of up to five components. 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's System Knowledge Base** contains data on over 600 pure components, 70 mixtures, and 80 physical property estimation techniques. You may find that this database is sufficient for most of your physical property data needs. However, Cranium's capabilities go far beyond a simple database program.

**Enter the Mixture's Surface Tension**

**Composition**

A:	Formic acid	38.0	wt %
B:	Water	62.0	wt %
C:	---		wt %
D:	---		wt %
E:	---		wt %

Clear   Rest   Units

**Data**

Temp: 298.15   Units: K

Datum: 0.0497   Units: N/m

Ref: Gammon93   List

OK  
OK & Next  
Cancel

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

**Enter the Material's Structure**

**Structural Items**

Element: Oxygen

Bond Type: Single Bond

**Options**

Subtractive Atoms

Automatic Bonding

Snap to Grid   Set

OK   OK & Next   Cancel

*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, materials, 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 material 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 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 tell Cranium to estimate a compound'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.

**Hf, 298 - Joback's Method**

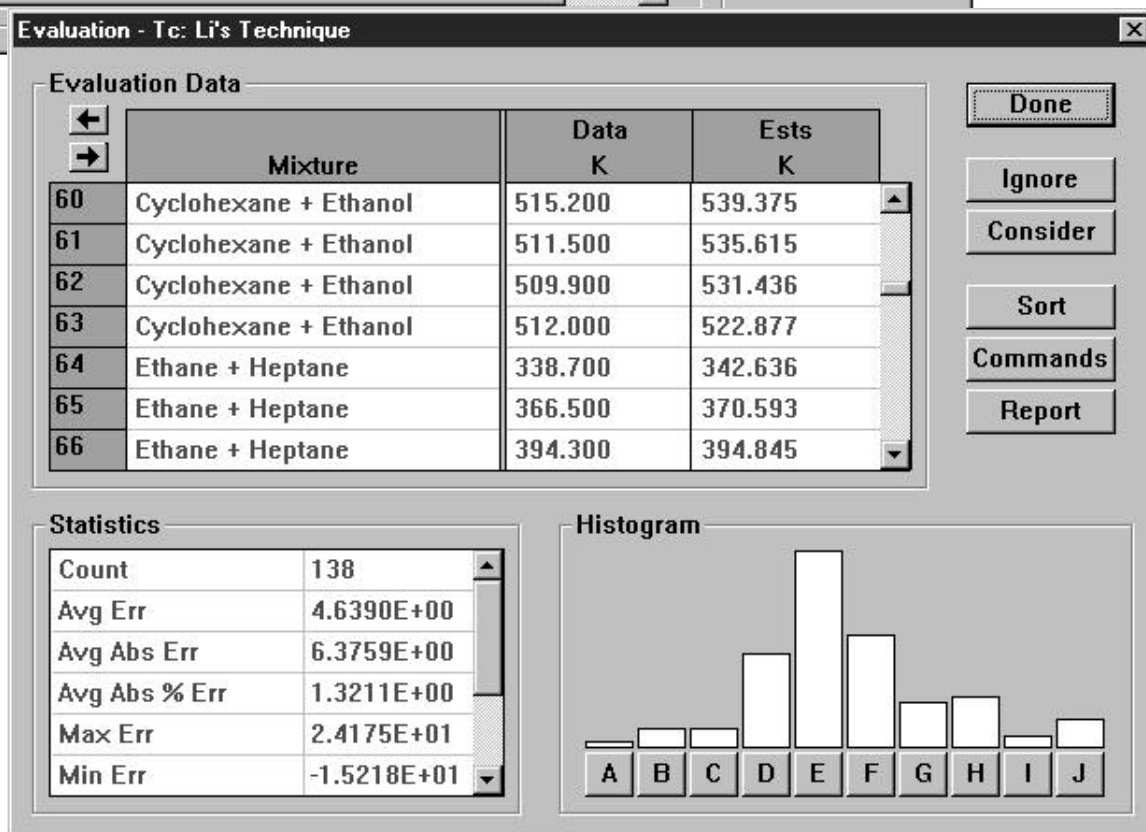
```
Code
// Dissect the material's structure
n = Dissect(material, technique, groups, occurs, err)
if( err != 0 ) return FALSE;

// Initialize contribution total
hf = 0.0;

// Total group contributions
for( i = 0; i < n; i = i + 1 )
{
    // Retrieve contribution
    con = Contribution(technique, groups[i], "", "");
    if( err != 0 ) return FALSE;
    hf = hf + con * occurs[i];
}
```

OK  
OK & Next  
Cancel  
Std Units  
Properties  
Functions  
Test

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



## KEY CAPABILITIES

- Automatically estimates over 20 physical properties
- Estimate a pure component's properties by simply drawing its molecular structure
- Estimate a mixture's properties by simply entering its composition
- Import molecular structures from MOL files
- Export property estimates to simulation programs
- Enter your own proprietary data and estimation techniques
- Create and distribute your own physical property databases
- Copy and paste physical properties into your favorite Windows programs

## PROPERTIES ESTIMATED

- Absolute Entropy
- Acentric Factor
- Activity Coefficient
- Boiling Point
- Critical Pressure
- Critical Temperature
- Critical Volume
- Densities
- Enthalpy of Formation
- Enthalpy of Vaporization
- Flash Point
- Freezing Point
- Gibbs Energy of Formation
- Heat Capacities
- Lower Flammability Limit
- Molecular Weight
- Surface Tension
- Thermal Conductivities
- Upper Flammability Limit
- Vapor Pressure
- Viscosities

## SYSTEM REQUIREMENTS

- Windows 95 or NT
- Mouse
- 16 MB RAM
- 15 MB Disk Space

FOR FURTHER  
INFORMATION AND  
A DEMONSTRATION  
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