

# CRANIUM<sup>®</sup>

*FAST,  
ACCURATE,  
AND EASY  
PHYSICAL  
PROPERTY  
ESTIMATION*

The screenshot shows the Cranium software window titled 'Common.mkskb'. The 'Mixtures' tab is selected, and the mixture '1,4-Dioxane + Propane' is displayed. The 'Constant Properties' section is active, showing the property 'Critical Temperature - f(X)' with the 'Estimates' method selected. A table displays the results for various compositions:

	X,1: 1,4-Dioxa...	X,2: Propane	X,3: ---	Ests
	mol %	mol %	mol %	K
1	18.2000	81.8000	---	414.7518
2	29.7000	70.3000	---	441.7598
3	43.7000	56.3000	---	473.2948
4	55.9000	44.1000	---	499.6430
5	66.7000	33.3000	---	522.1382
6	68.9000	31.1000	---	526.6287
7	86.9000	13.1000	---	562.2567
8	---	---	---	---

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*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, organometallics, 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.

Enter the Mixture's VLE, Bubble Point - f(T,P,X) (Modified)

Equilibrium Composition Units: **mol frac**

Ammonia	X:	0.1494	±	
Water	X:	0.8133	±	
Lithium Bromide	X:	0.0373	±	

Equilibrium Pressure and Temperature

Temp: 333.17 ± Units: **K**

Pres: 100 ± Units: **kPa**

Source Information

Reference: **Peters-Greb-Korinth-Zimmermann-Keller** List

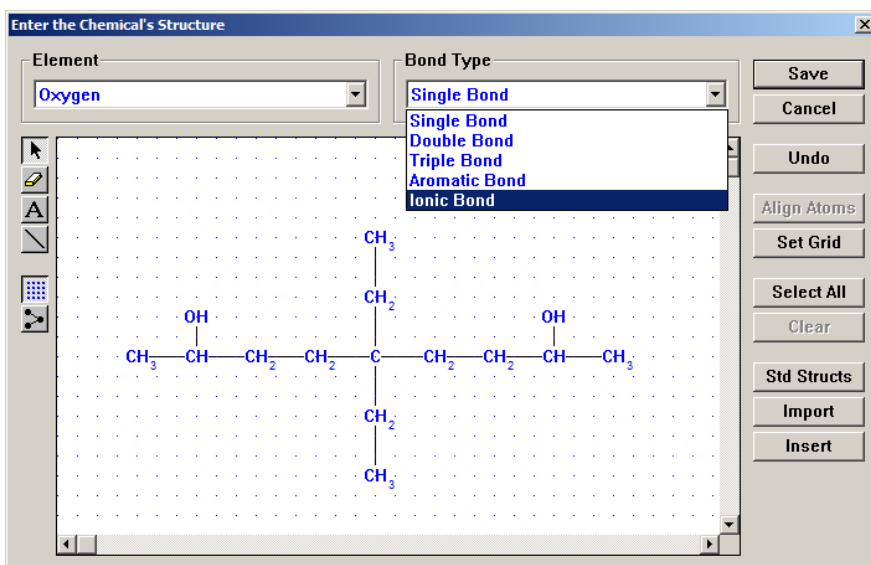
Comment:

Nov 12, 2008 at 15:13:49, MKS-KGJ  
Entered and verified.

Date Phrase Set

OK  
OK & Next  
Cancel  
X Default  
X Total

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*

The screenshot displays the Cranium software interface. At the top, a window titled "Enter Estimation Code for Tc: Joback's Method" contains a code editor with the following C-like code:

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

    // Total contribution
    total = total + contrib * occurs[i];
}

// Add the terms
den = 0.584 + 0.965 * total - total * total;

// Compute the final estimate
tc = tb / den;
```

Below the code editor are buttons for "Save", "Cancel", "Default Args", "Properties", "Std Units", and "Test". To the right of the code editor is a text box with the instruction: "You can enter your own proprietary estimation techniques or modify any of Cranium's techniques".

Below the code editor is a window titled "Function Example and Documentation" with a list of functions: cubic, Dissect, double, Elements, else, EProp, exp, FALSE.

The main window is titled "Evaluation of Tc: Joback's Method" and contains an "Evaluation Records" table:

	Name	---	Data	Ests	
	---	---	K	K	
29	2,2,4-Trimethylpentane	---	543.9600	547.7079	3.74
30	2,2,5-Trimethylhexane	---	568.0000	572.7757	4.77
31	2,2-Dimethylbutane	---	488.7800	491.8907	3.11
32	2,2-Dimethylheptane	---	576.8000	580.9268	4.12
33	2,2-Dimethylhexane	---	549.8700	554.5235	4.65

Below the table is a "Statistics" window with the following data:

Statistic	Value
# Observations	192
Avg Error	-1.9886
Avg Abs Error	6.1116
Avg Abs % Error	1.1614
Max Error	59.1627
Min Error	-144.5701
Max Abs Error	16.8810
Min Abs Error	1.1369E-13

To the right of the statistics is a "Graph" window showing a scatter plot of "Estimates" vs "Data" with a blue regression line. The plot shows a strong positive linear correlation between the data points and the estimates.

At the bottom right of the main window are buttons for "Done", "Consider", "Ignore", "Copy All", and "Sort".

## KEY CAPABILITIES

- Automatically estimate over 50 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
- Acid Dissociation Constant
- Activity Coefficient
- Acute Toxicity
- Aquatic Toxicity
- Autoignition Temperature
- Bioconcentration Factor
- Biological Oxygen Demand
- Boiling Point
- Chemical Oxygen Demand
- Critical Pressure
- Critical Temperature
- Critical Volume
- Densities
- Diffusion Coefficients
- Enthalpy of Formation
- Enthalpy of Fusion
- Enthalpy of Vaporization
- Flash Point
- Freezing Point
- Fugacity Coefficient
- Gibbs Energy of Formation
- Heat Capacities
- Henry's Law Constant
- Liquid-Liquid Equilibria
- Lower Flammability Limit
- Melting Point
- Molecular Weight
- Octanol-Water Partition
- Refractive Index
- Second Virial Coefficient
- Solid-Liquid Equilibria
- Solubility Parameter
- Speed of Sound
- Surface Tension
- Thermal Conductivities
- Triple Point Pressure
- Triple Point Temperature
- Upper Flammability Limit
- Vapor Pressure
- Vapor-Liquid Equilibria
- Viscosities
- Water Solubility

TO RECEIVE MORE  
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