For inquiries, please contact us at staff@chemessen.com

ChemEssen, Inc.
1408, AceHighTechCity 2-Cha, 25 Seonyu-ro 13-gil,
Yeongdeungpo-gu,07282 Seoul, Republic of Korea
Tel: +82.2.3143.5933 I Fax: +82.2.3143.5920
www.chemessen.com

IK-CAPE File

Provided By

ChemEssen, Inc.

Over 5 Million IK Cape Files

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About Our IK-CAPE File

IK-CAPE files (*.IKC) are specialized text-based data files containing thermophysical property information, specifically designed for use with process simulation software such as Aspen Technology's Aspen Plus®. These files comply with the CAPE-OPEN standard, ensuring seamless compatibility across various process simulation platforms.

IK-CAPE files are indispensable when using process simulation software, such as Aspen Plus®. A common challenge arises when the software's built-in component database lacks the desired compound. This limitation can halt simulations, making it difficult to proceed. With our IK-CAPE files, you can seamlessly integrate additional compounds into your simulation, allowing you to proceed without interruptions.

Our IKC file contains the following data:

NO	Symbol	Meaning
1	MW	Molecular Weight
2	OMEGA	Acentric Factor
3	ZC	Critical Compressibility Factor
4	TC	Critical Temperature
5	PC	Critical Pressure
6	VC	Critical Volume
7	DIPM	Dipole Moment
8	HLSM	Heat of Melting at Normal Melting Point
9	VOL0	Volume at Standard Conditions
10	TB	Normal Boiling Point (1 atm)
11	RGYR	Radius of Gyration

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12	S0V	Standard Entropy (Vapor)
13	S0L	Standard Entropy (Liquid)
14	S0S	Standard Entropy (Solid)
15	HF0V	Standard Heat of Formation (Vapor)
16	HF0L	Standard Heat of Formation (Liquid)
17	HF0S	Standard Heat of Formation (Solid)
18	GF0V	Standard Free Energy of Formation (Vapor)
19	GF0L	Standard Free Energy of Formation (Liquid)
20	GF0S	Standard Free Energy of Formation (Solid)
21	PARA	Parachor
22	HLVB	Heat of Vaporization at Normal Boiling Point
23	CPIG	Heat Capacity of Ideal Gas
24	CP (V, L)	Heat Capacity (Vapor, Liquid)
25	HLV	Heat of Vaporization
26	DEN (L)	Density (Liquid)
27	SFTN	Surface Tension
28	K (V, L)	Thermal Conductivity (Vapor, Liquid)
29	PVL	Vapor Pressure
30	VIS (V, L)	Viscosity (Vapor, Liquid)
31	VIR2	Second Virial Coefficient
32	RINAD	Refractive Index, Na-D-Line
33	PTCOW	Octanol/Water Partition Coefficient
34	SOLW	Solubility within Water
35	HF (V, L)	Heat of Formation (Vapor, Liquid)
36	H (V, L)	Enthalpy (Vapor, Liquid)
37	S (V, L)	Entropy (Vapor, Liquid)
38	G (V, L)	Gibbs Energy (Vapor, Liquid)
39	GF (V, L)	Gibbs Energy of Formation (Vapor, Liquid)

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A Step-by-Step Example

Importing IK-CAPE Files & Estimating Binary Interaction Parameters in Aspen Plus®

This guide demonstrates how to import IK-CAPE files into Aspen Plus®, set up molecular structures using SMILES strings, and calculate binary interaction parameters for process simulations. This example is particularly useful when your desired compound is missing from Aspen Plus's built-in component database.

In this example, we'll use two compounds not currently included in Aspen Plus®:

- (2Z)-2-ethylbut-2-en-1-ol
- (2R)-1,1,2-trimethylcyclopropane

You can download the IK-CAPE files here:

Download IKC File Examples

Once downloaded, extract the ZIP file to access the two IK-CAPE files and their respective SMILES string files (*.smi).

The process involves three main steps:

1. Importing IK-CAPE Files into Aspen Plus®
2. Setting Up Molecular Structures Using SMILES Strings

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3. Setting Up Simulation Methods and Estimating Binary Interaction Parameters

1. Importing IK-CAPE Files into Aspen Plus®

To import IK-CAPE files into an opened simulation, follow these steps:

(1) Click **File (Top Menu)** > **Import (Left Panel Menu)** > **File (Right Panel Menu)**.
(2) Select File Type: **IK-CAPE Files (*.ikc)**.
(3) Navigate to the folder where the IKC files are located.
(4) Select the first IKC file and click **Open**.
(5) Repeat steps 1–4 for the second IKC file.
(6) When the "Resolve ID Conflicts" window appears, click object **Properties Parameters...**
(7) Click **Merge (Right Panel Menu)** > Click **OK (Right Panel Menu)**.
(8) Warning Message Appears, **Warning! If merged items...** > Click **OK**.
(9) Remove Component Name (Aspen's incorrect assignment): Right click of the mouse and select **Clear**.
(10) Verify the imported files: Unfold **Methods (Left Panel Menu) > Unfold "Parameters** > Unfold **Pure Components** > Click **PD-1**.

2. Setting Up Molecular Structures Using SMILES Strings

This step configures the molecular structure of the imported IKC files:

(1) Unfold **Components (Left Panel Menu)** > **Molecular Structure** : Two Imported IKC components are shown.
(2) Click the first IKC component > Click **Structure and Functional Group** (Right Panel Tab).
(3) Click **Draw/Import/Edit** button on the left > Molecule Editor Window appears.
(4) Click the folder icon in the editor (first icon on the top left)
(5) Select the corresponding *.smi file > Click **Open** button > The molecular structure appears.

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(6) Close the Molecule Editor Window by clicking the "x" button on the top right > Verify the molecular structure on the graphical structure box on the left.
(7) Click **Calculate Bonds** button on the left to complete the structure setup.
(8) Click the **General** Tab > Verify the atom & bond type
(9) Repeat steps 2–8 for the second IKC component.

3. Setting Up Simulation Methods and Binary Interaction Parameter Estimation

This step sets up the binary interaction parameter estimation for the imported IK-Cape files using Aspen Plus' R-PCES method:

(1) Click **Methods (Left Panel Menu)** > **Specifications**
(2) Click **Global Tab** > **Base method**
(3) Select a method, e.g., **NRTL** (You can choose different method)
(4) Unfold **Binary Interaction (Left Panel Menu)**
(5) Click **NRTL-1** > Confirm BIPs are initially empty .
(6) Click **Estimation (Left Panel Menu)** > Under **Setup tab**, select **Estimate all missing parameters**
(7) Click **Binary** tab > Click "**New**" button
(8) Click **Parameter** on the left to choose NRTL (This method was determined in the step (3) above)
(9) Click **Method** and select **UNIF-DMD** (You can choose different group contribution method)
(10) Click **Component i** and select the first IK-Cape component > Click **Component j** and select the second IK-Cape component
(11) Enter the first temperature approximately using the lower boiling point between the two IK-Cape components in Celsius (Obtain the boiling points from **Method > Parameters > Pure Components > PD-1 > TB (Left Panel Menu**. In the case of the imported IK-Cape files in this example, enter 328.942 – 273.15 = ~55)

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(12) Enter the second temperature approximately using the higher boiling point between the two IK-Cape components in Celsius. (Obtain the boiling points from **Method > Parameters > Pure Components > PD-1 > TB (Left Panel Menu**. In the case of the imported IK-Cape files in this example, enter 423.928 – 273.15 = ~150)

(13) Click **Methods (Left Panel Menu)** > **Parameters** > **Binary Interaction** > **NRTL-1** and confirm currently Binary Interaction Parameters are empty

(14) Click **Run (Top Menu)** > Confirm the Binary Interaction Parameters are now estimated.

(15) Click **Binary (Top Menu)** graph button > Click **Calculation Options** Tab > Change **Maximum iteration** to 100

(16) Click **Binary Analysis** Tab> Click **Run Analysis (Bottom Menu)** Button

(17) Confirm a reasonable T-xy graph.