

Specification for the CPI Component Data File Format Version 2.0 Revised: 25/02/2011

Introduction

This document provides a specification for the University of Manchester Centre for Process Integration (CPI) Data File (CMP File) format. The CMP file format is a proprietary format, containing a list of components and physical properties, together with the parameters required to calculate those properties.

The physical property algorithms themselves are encoded into the CPI's suite of process integration software. The purpose of the CMP file is to provide a consistent mechanism whereby the components and parameters can be imported into CPI's software.

A CMP file contains:

- A list of chemical components
- A list of physical properties (e.g. enthalpy, vapour pressure)
- A list of methods, used to calculate the physical properties
- A list of parameters which are required for calculation of the property, using the specified method

CMP files are currently created using Component Editor (CmpEdit), a file editor supplied with CPI's software.

The purpose of this document is to provide sufficient information to enable third parties to produce CMP files which are compatible CPI's software. In particular it enables the writing of macros which automatically export the data from commercial simulators.

Basic Principles

The basic properties of the CMP file are:-

- Free-format ASCII
- Case insensitive
- Order insensitive (within each section)

The file consists of the following three sections

- **Headers:** This must be the first section in the file, and contains the version number of the data file, and optional information regarding the source of the data.

- **Counters:** This must precede the Data section, and provides summary information regarding the number of components and properties that follow in the file. The start of the Counters section is identified in the file by the single line:

[COUNTERS]

- **Data Section:** The Data section must follow the Counters section, and contains all the information and parameters relating to the components and properties introduced in the Counters section. The start of the Data section is identified in the file by the single line:

[DATA]

Within each section, information is supplied in the form:

Item_Name = value_1, value_2, value_3..., value_n

Where **Item_Name** is a unique keyword, followed by a list of values separated by commas. The values may be of type integer, real or character, and must all be on the same line as the keyword. The number and type of values associated with each keyword is fixed, and defined below.

Comments may be freely used anywhere within the file by including “[###” or “!” as the first characters on the line, e.g.

[### this is a comment]

! This is also a comment

In-line comments may be included with the “;” character. Any text following the “;” character is ignored, for the rest of the line, e.g.

NUM_Components = 5 ; Comment – 5 components in file

Keywords

The following is a complete list of the keywords recognised for use in a CMP file. Each keyword must appear in its respective section (Headers, Counters or Data). Any keyword that is not in the correct section, or is not recognised, will be ignored without affecting the validity of the rest of the file.

Each keyword is specified as follows

KeyWord = <value_1>, <value_2>, ... <value_n>

The type of each value is indicated

<n> = Integer
<r> = Real

<string> = Character string

Headers Section

The first line of the header must consist of the current version number, followed by optional reference information, for example:

2.0 [UMIST CMP Data File Version Number 02/11/1998 10:34:00]

The CMP file is currently at version 2.0

The following optional keywords may be included in the headers, but are not required:

Inf_Program_Name = <string>
where <String> is the source of the data

Inf_Program_Version = <n>
where <n> is the version number of the data source

Inf_Program_Build_Date = <n>
where <n> is the date of file creation

Counters Section Section

The following keywords and associated values are required in the Counters section of the file. Note that all counter keywords begin with the prefix **NUM_**

NUM_Components = <n>
Number of components
<n> is the number of components present in the file

NUM_Properties = <n>
Number of properties
<n> is the number of properties within the file. See Appendix A for a full list of available properties.

NUM_CompID = <n1>, <n2>
Component ID number
<n1> is the ordinal number of the component within the file
<n2> is a unique identification number (ID number) for the component. Throughout the entire file each component is referenced by its ID number.

NUM_PropID = <n1>, <n2>
Property reference number
<n1> is the ordinal number of the property within the file
<n2> is the reference number of the component. See Appendix A for a list of property reference numbers.

Data Section

The following keywords and associated values are required in the Data section of the file. Note that all counter keywords begin with the prefix **PPD_**. If all of the values associated with a particular keyword are equal to 0.0, the keyword may be omitted from the file.

PPD_LongName = <n>, <string>

Component long name

<n> is the ID number of a component

<string> is a long name for the component. The name may be up to 40 characters long

PPD_ShortName = <n>, <string>

Component short name

<n> is the ID number of a component

<string> is a short name (e.g. formula) for the component. The name may be up to 15 characters long

PPD_PropertyMethod = <n1>, <n2>

Method used to calculate a property

<n1> is the reference number of the property

<n2> is the method number for the property. See Appendix A for a list of property reference and method numbers.

PPD_CriticalData = <n>, <r1>, <r2>, <r3>, <r4>, <r5>, <r6>, <r7>, <r8>, <r9>

Critical data for a component

<n> is the ID number of the component

<r1> is the molecular weight, MolWt, (g/mol)

<r2> is the normal freezing point at 1 atmosphere, Tfp, (Kelvin)

<r3> is the normal boiling point at 1 atmosphere, Tb, (Kelvin)

<r4> is the critical temperature, Tc, (K)

<r5> is the critical pressure, Pc, (Bar)

<r6> is the critical volume, Vc, (cm³/mole)

<r7> is the critical compressibility factor, Zc (PcVc/RTc)

<r8> is Pitzer's acentric factor

<r9> is the dipole moment, (debyes)

PPD_CriticalDat2 = <n>, <r1>, <r2>, <r3>, <r4>, <r5>, <r6>, <r7>, <r8>, <r9>

Critical data for a component

c PURE_PROP_DN = density at std condition (kg/m³) - maybe

<n> is the ID number of the component

<r1> is the solubility, SI (????)

<r2> is Molar Volume, Mv, (cm³/mol)

<r3> is the Non-condensable flag, (0/1)

<r4> is the density at standard condition, Dn, (kg/m³)

<r5> reserved for future use

<r6> reserved for future use

<r7> reserved for future use

<r8> reserved for future use

<r9> reserved for future use

PPD_PropParam = <n1>, <n2>, <n3>, <r>

Parameters for a component/property pair. The number of parameters for each component/property pair depends on the method being used to calculate the property.

<n1> is the reference number of the property

<n2> is the ID number of the component

<n3> is the parameter number

<r> is the value of the parameter. See Appendix A for a list of parameters required for

each property/method combination

PPD_InterParam = <n1>, <n2>, <n3>, <r1>, <r2>

Binary interaction parameters for a component pair (only required when the Activity Coefficients property is present)

<n1> is the ID number of the first component in the pair

<n2> is the ID number of the second component in the pair

<n3> is the number of binary matrix. (Refer to Appendix A for details of which binary matrices are required for each Activity Model.)

<r1> is the value of the interaction parameter for component pair <n1>, <n2>

<r2> is the value of the interaction parameter for component pair <n2>, <n1>

Example:

PPD_InterParam = 77, 170, 1, 904.77, -14.583

Indicates that:

$$A_{i,j} = 904.77$$

$$A_{j,i} = -14.583$$

i is the component with ID number 77

j is the component with ID number 170

Appendix A: Physical Properties and Methods

This appendix describes the primary physical property routines and methods that are available in the CPI's software.

Where a property/method pair requires additional parameters, the form of the equation used is supplied. If a property requires no additional parameters, the form of the equation is not required to produce a CMP file, and is not supplied. This keeps the amount of information supplied to a bare minimum.

The available property list currently comprises three core properties (enthalpy, vapour pressure and equation of state), an activity model, and several further optional properties. The optional properties are only required in a small class of calculations, and are not included in this version of the specification.

A CMP file must always contain the three core properties as a minimum. The activity model is optional. If the activity model is present it will be used for calculating liquid phase properties, with the selected equation of state being used for vapour phase calculations only.

The properties and methods are summarised in the following table

Property Name	Reference Number	Available Methods	Required
Enthalpy	2	1: Reid, Prausnitz, Poling 2: DIPPR 3. Hysys-Tabular 4. Lee-Kesler	Yes
Vapour Pressure	3	1: Reid, Prausnitz, Poling 2: Dechema 3: Extended Antoine (HYSYS) 4: Extended Antoine (AspenTech)	Yes
Equation of State	11	1: Ideal Gas (Raoult's Law) 2: Peng-Robinson 3: Soave-Redlich-Kwong (SRK) 4: Grayson-Streed	Yes
Activity Model	9	1: Wilson 2: NRTL 3: UNIQUAC 4: Extended NRTL (AspenTech)	No

Enthalpy

Method 1: Reid-Prausnitz-Poling

This method uses a standard third order polynomial to calculate the heat capacities, and integrates with respect to temperature to calculate the enthalpies.

The equation used to calculate the heat capacities is:

$$C_p = A + BT + CT^2 + DT^3$$

Where C_p = heat capacity of the ideal gas, J/(mol.K)

T = Temperature, K

The parameters required on the respective **PPD_PropParam** keyword are:

Parameter Number	Parameter Name	Parameter Symbol/Description
1	CPVAP A	A
2	CPVAP B	B
3	CPVAP C	C
4	CPVAP D	D

Ref. The Properties of Gases and Liquids, 4th Edition, Reid, Prausnitz and Poling, p.657

Method 2: DIPPR

This method uses the DIPPR ideal gas heat capacity equation, and integrates with respect to temperature to calculate the enthalpies.

The equation used to calculate the heat capacities is:

$$C_p = C_1 + C_2 \left(\frac{C_3/T}{\sinh(C_3/T)} \right)^2 + C_4 \left(\frac{C_5/T}{\cosh(C_5/T)} \right)^2 \text{ for } T_{\min} \leq T \leq T_{\max}$$

Where C_p = heat capacity of the ideal gas, J/(mol.K)

T = Temperature, K

The parameters required on the respective **PPD_PropParam** keyword are:

Parameter Number	Parameter Name	Parameter Symbol/Description
1	CPVAP A	C_1
2	CPVAP B	C_2
3	CPVAP C	C_3
4	CPVAP D	C_4
5	CPVAP E	C_5
6	Tmin	Lower temperature limit (K)

7	Tmax	Upper temperature limit (K)
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Ref AspenTech User Guide V10.2, Physical Property Methods and Models, p3-109

Method 3: Hysys Tabular

Method 4: Les-Kesler

This method uses a standard third order polynomial to calculate the enthalpies, and differentiates with respect to temperature to calculate the heat capacities

The equation used to calculate the enthalpies is:

$$H = A + B*T + C*(T^2) + D*(T^3) + E*(T^4)$$

Where:-

H = Enthalpy of ideal gas at temperature T [kJ/kg]

T = Temperature [K]

The parameters required on the respective **PPD_PropParam** keyword are:

Parameter Number	Parameter Name	Parameter Symbol/Description
1	CPVAP A	A
2	CPVAP B	B
3	CPVAP C	C
4	CPVAP D	D
5	CPVAP E	E

(Ref: HYSIM Ver.2.10 User's Guide, 1993, pp.5-29)

Vapour Pressure

Method 1: Reid-Prausnitz-Poling

This method uses one of three equations to calculate vapour pressure, as follows:

$$\text{Eqn (1)} \quad \ln(P_{vp}/P_c) = (1-x)^{-1} [(VP A)x + (VP B)x^{1.5} + (VP C)x^3 + (VP D)x^6]$$

$$x = 1 - T/T_c$$

$$\text{Eqn (2)} \quad \ln(P_{vp}) = VP A - (VP B)/T + (VP C) \ln T + (VP D)(P_{vp})T^2$$

$$\text{Eqn (3)} \quad \ln(P_{vp}) = VP A - (VP B)/(T + (VP C))$$

Where P_{vp} = Vapour pressure, bars

P_c = Critical pressure, bars

T_c = Critical temperature, K

T = Temperature, K

The parameters required on the respective **PPD_PropParam** keyword are:

Parameter Number	Parameter Name	Parameter Symbol/Description
1	Eqn. No.	Equation number
2	VP A	$VP A$
3	VP B	$VP B$
4	VP C	$VP C$
5	VP D	$VP D$
6	Tmin	Lower temperature limit (K)
7	Tmax	Upper temperature limit (K)

Ref. The Properties of Gases and Liquids, 4th Edition, Reid, Prausnitz and Poling, p.657

Method 2: DECHEMA

This method uses a DECHEMA correlation of the Antoine equation. The equation is as follows

$$\ln(P_{vp}) = A - \frac{B}{T + C}$$

Where P_{vp} = Vapour pressure, bars

T = Temperature, K

The parameters required on the respective **PPD_PropParam** keyword are:

Parameter Number	Parameter Name	Parameter Symbol
1	Antoine A	A
2	Antoine B	B

3	Antoine C	C
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Ref. The Properties of Gases and Liquids, 4th Edition, Reid, Prausnitz and Poling,
p.208

Method 3: Modified Antoine (HYSYS)

This method uses a modified version of the Antoine equation, as used in the Hyprotech HYSYS simulator. The equation is:

$$\ln(P_{vp}) = A + \left(\frac{B}{T+C} \right) + D \ln(T) + ET^F$$

Where P_{vp} = Vapour pressure, kPa
 T = Temperature, K

The parameters required on the respective **PPD_PropParam** keyword are:

Parameter Number	Parameter Name	Parameter Symbol
1	Antoine A	<i>A</i>
2	Antoine B	<i>B</i>
3	Antoine C	<i>C</i>
4	Antoine D	<i>D</i>
5	Antoine E	<i>E</i>
6	Antoine F	<i>F</i>

Ref. HYSYS User documentation v2.4.1

Method 4: Modified Antoine (Aspen)

This method uses a modified version of the Antoine equation, as used in the AspenTech AspenPlus simulator. The equation is:

$$\ln(P_{vp}) = A + \left(\frac{B}{T+C} \right) + DT + E \ln(T) + FT^G \quad \text{for } T_{\min} \leq T \leq T_{\max}$$

Where P_{vp} = Vapour pressure, bars
 T = Temperature, K

The parameters required on the respective **PPD_PropParam** keyword are:

Parameter Number	Parameter Name	Parameter Symbol
1	Antoine A	<i>A</i>
2	Antoine B	<i>B</i>
3	Antoine C	<i>C</i>
4	Antoine D	<i>D</i>
5	Antoine E	<i>E</i>
6	Antoine F	<i>F</i>
7	Antoine G	<i>G</i>
8	Tmin	Lower temperature limit (K)
9	Tmax	Upper temperature limit (K)

Ref AspenTech User Guide V10.2, Physical Property Methods and Models, p3-84

Equation of State

Method 1: Ideal Gas (Raoult's Law)

There are no additional parameters associated with the Ideal equation of state.

Method 2: Peng-Robinson

There are no additional parameters associated with the Peng-Robinson equation of state.

Method 3: Soave-Redlich-Kwong (SRK)

There are no additional parameters associated with the SRK equation of state.

Method 4: Grayson-Streed

There are no additional parameters associated with the grayson-streed equation of state.

Activity Models

Activity models use one or more matrices of binary parameters, and in the case of the UNIQUAC model, two further component specific parameters.

Because parameters are required for each component pair, rather than for each individual component, a separate keyword is used to supply the parameters.

Method 1: Wilson

This method uses the standard Wilson equation to calculate activity coefficients. The form of the equation is:

$$\ln \gamma_i = -\ln \left(\sum_j^N x_j \Lambda_{ij} \right) + 1 - \sum_k^N \frac{x_k \Lambda_{ki}}{\sum_j^N x_j \Lambda_{kj}}$$

Where γ_i = activity co-efficient for component i

Λ_{ij} = $V_j/V_i \exp(-a_{ij}) / RT$

a_{ij} = binary interaction parameters for component pair i, j

V_i = molar volume of pure liquid component i in m^3/kgmol

The parameters required on the respective **PPD_InterParam** keyword are:

Binary Matrix No.	Interaction Parameters
1	a_{ij}

The parameters required on the respective **PPD_PropParam** keyword are:

Parameter Number	Parameter Name	Parameter Symbol/Description
1	Mol. Vol.	Molar volume, m^3/kgmole

Method 2: NRTL

This method uses the standard NRTL equation to calculate activity coefficients. The form of the equation is:

$$\ln \gamma_i = \frac{\sum_j^N \tau_{ji} G_{ji} x_j}{\sum_k^N G_{ki} x_k} + \sum_j^N \frac{x_j G_{ij}}{\sum_k^N G_{kj} x_k} \left(\tau_{ij} - \frac{\sum_k^N x_k \tau_{kj} G_{kj}}{\sum_k^N G_{kj} x_k} \right)$$

Where γ_i = activity co-efficient for component i

τ_{ij} = a_{ij} / RT

G_{ij} = $\exp(-\alpha_{ij} \tau_{ij})$

a_{ij}, α_{ij} = two pairs of binary interaction parameters for component pair i, j ($\alpha_{ij} = \alpha_{ji}$)

The parameters required on the respective **PPD_InterParam** keyword are:

Binary Matrix No.	Interaction Parameters
1	a_{ij}, a_{ji}
2	α_{ij}, α_{ji}

Note that because $\alpha_{ij} = \alpha_{ji}$. The keyword entry for the α matrix should contain identical values for the two parameters, e.g.

PPD_InterParam = 77, 170, 2, 0.295, 0.295 ; α_{ij} and α_{ji} for $i = 77, j = 170$

Method 3: UNIQUAC

This method uses the UNIQUAC equation to calculate activity coefficients. The form of the equation is:

$$\ln \gamma_i = \ln \frac{\Phi_i}{x_i} + \frac{z}{2} q_i \ln \frac{\theta_i}{\Phi_i} + l_i - \frac{\Phi_i}{x_i} \sum_j x_j l_j - q_i \ln \left(\sum_j \theta_j \tau_{ji} \right) + q_i - q_i \sum_j \frac{\theta_j \tau_{ij}}{\sum_k \theta_k \tau_{kj}}$$

Where $\Phi_i = \frac{r_i x_i}{\sum_k r_k x_k}$

$$\theta_i = \frac{q_i x_i}{\sum_k q_k x_k}$$

$$\tau_{ij} = \exp(a_{ij} / RT)$$

r_i = molecular-size parameter for component i

q_i = molecular-surface parameter for component i

The parameters required on the respective **PPD_InterParam** keyword are:

Binary Matrix No.	Interaction Parameters
1	a_{ij}

The parameters required on the respective **PPD_PropParam** keyword are:

Parameter Number	Parameter Name	Parameter Symbol/Description
1	r_i	r_i
2	q_i	q_i

Method 4: NRTL (AspenTech)

This method uses an extended version of the NRTL equation as used in the AspenTech AspenPlus simulator. The form of the equation is:

$$\ln \gamma_i = \frac{\sum_j^N \tau_{ji} G_{ji} x_j}{\sum_k^N G_{ki} x_k} + \sum_j^N \frac{x_j G_{ij}}{\sum_k^N G_{kj} x_k} \left(\tau_{ij} - \frac{\sum_k^N x_k \tau_{kj} G_{kj}}{\sum_k^N G_{kj} x_k} \right)$$

Where γ_i = activity co-efficient for component i

$$\tau_{ij} = a_{ij} + (b_{ij}/T) + e_{ij} \ln(T) + f_{ij} T$$

$$G_{ij} = \exp(-\alpha_{ij} \tau_{ij})$$

$$\alpha_{ij} = c_{ij} + d_{ij}(T - 273.15K)$$

a_{ij} to f_{ji} = six pairs of binary interaction parameters for component pair i, j (c_{ij} = c_{ji} and d_{ij} = d_{ji})

The parameters required on the respective **PPD_InterParam** keyword are:

Binary Matrix No.	Parameter Name
1	a_{ij}, a_{ji}
2	b_{ij}, b_{ji}
3	c_{ij}, c_{ji}
4	d_{ij}, d_{ji}
5	e_{ij}, e_{ji}
6	f_{ij}, f_{ji}

Note that because $c_{ij} = c_{ji}$ and $d_{ij} = d_{ji}$ the keyword entry for the c and d matrices should contain identical values for the two parameters, e.g.

170 **PPD_InterParam** = 77, 170, 3, 140.3, 140.3 ; c_{ij} and c_{ji} for $i = 77, j =$

170 **PPD_InterParam** = 77, 170, 4, -254.5, -254.3 ; d_{ij} and d_{ji} for $i = 77, j =$

Additional data elements

This is optional data can be stored in the .CMP file that is only used by CmpEdit and is not used by the general physical properties calculation engines.

Physical properties calculator

Stream conditions

PPC_Z = <n>, <r1>

Profile pressure

<n> is the component index

<r1> is the component mole fraction

PPC_FLOW = <r1>

<r1> is the fluid flowrate (kmole/s)

PPC_P = <r1>

<r1> is pressure (bar)

PPC_T_K = <r1>

<r1> is the temperature (Kelvin)

PPC_H = <r1>

<r1> is the specific enthalpy (kJ/kmole)

PPC_S = <r1>

<r1> is the specific entropy (Kw/K)

PPC_VF = <r1>

<r1> is the vapour fraction

PPC_Property = <n>

<n> is the index of the property to be calculated

PPC_Range_BL = <r1>

<r1> range calculation lower bound

PPC_Range_BU = <r1>

<r1> range calculation upper bound

Profile properties

PPC_ENV_T_Min_K = <r1>

PPC_ENV_T_Max_K = <r2>

PPC_ENV_Num_P = <n>

PPC_ENV_Num_Plot_Points = <n>

PPC_ENV_P = <n>, <r1>

<n> is the component index

<r1> is the profile pressure (bar)


```

PPD_CriticalDat2 = 311, 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000
, 0.000000
PPD_CriticalDat2 = 258, 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000 , 0.000000
, 0.000000

[### Physical Property Parameters (Property, Component ID, Parameter Number, Value)]

[### Enthalpy parameters for i-butane]
PPD_PropParam = 2, 259, 1, -1.3900000
PPD_PropParam = 2, 259, 2, 0.38470000
PPD_PropParam = 2, 259, 3, -0.18500000E-03
PPD_PropParam = 2, 259, 4, 0.28950000E-07

[### Enthalpy parameters for propane]
PPD_PropParam = 2, 206, 1, -4.2240000
PPD_PropParam = 2, 206, 2, 0.30630000
PPD_PropParam = 2, 206, 3, -0.15900000E-03
PPD_PropParam = 2, 206, 4, 0.32150000E-07

[### Enthalpy parameters for i-pentane]
PPD_PropParam = 2, 312, 1, -9.5250000
PPD_PropParam = 2, 312, 2, 0.50660000
PPD_PropParam = 2, 312, 3, -0.27300000E-03
PPD_PropParam = 2, 312, 4, 0.57230000E-07

[### Enthalpy parameters for n-pentane]
PPD_PropParam = 2, 311, 1, -3.6260000
PPD_PropParam = 2, 311, 2, 0.48730000
PPD_PropParam = 2, 311, 3, -0.25800000E-03
PPD_PropParam = 2, 311, 4, 0.53050000E-07

[### Enthalpy parameters for n-butane]
PPD_PropParam = 2, 258, 1, 9.4870000
PPD_PropParam = 2, 258, 2, 0.33130000
PPD_PropParam = 2, 258, 3, -0.11100000E-03

[### Vapour Pressure parameters for i-butane]
PPD_PropParam = 3, 259, 1, 1.0000000
PPD_PropParam = 3, 259, 2, -6.9557900
PPD_PropParam = 3, 259, 3, 1.5000000
PPD_PropParam = 3, 259, 4, -2.5271700
PPD_PropParam = 3, 259, 5, -1.4577600
PPD_PropParam = 3, 259, 6, 165.00000
PPD_PropParam = 3, 259, 7, 408.20000

[### Vapour Pressure parameters for propane]
PPD_PropParam = 3, 206, 1, 1.0000000
PPD_PropParam = 3, 206, 2, -6.7221900
PPD_PropParam = 3, 206, 3, 1.3323600
PPD_PropParam = 3, 206, 4, -2.1386800
PPD_PropParam = 3, 206, 5, -1.3855100
PPD_PropParam = 3, 206, 6, 145.00000
PPD_PropParam = 3, 206, 7, 369.80000

[### Vapour Pressure parameters for i-pentane]
PPD_PropParam = 3, 312, 1, 1.0000000
PPD_PropParam = 3, 312, 2, -7.1272700
PPD_PropParam = 3, 312, 3, 1.3899600
PPD_PropParam = 3, 312, 4, -2.5430200
PPD_PropParam = 3, 312, 5, -2.4565700
PPD_PropParam = 3, 312, 6, 220.00000
PPD_PropParam = 3, 312, 7, 460.40000

[### Vapour Pressure parameters for n-pentane]
PPD_PropParam = 3, 311, 1, 1.0000000
PPD_PropParam = 3, 311, 2, -7.2893600
PPD_PropParam = 3, 311, 3, 1.5367900
PPD_PropParam = 3, 311, 4, -3.0836700
PPD_PropParam = 3, 311, 5, -1.0245600
PPD_PropParam = 3, 311, 6, 195.00000
PPD_PropParam = 3, 311, 7, 469.70000

[### Vapour Pressure parameters for n-butane]
PPD_PropParam = 3, 258, 1, 1.0000000
PPD_PropParam = 3, 258, 2, -6.8070900
PPD_PropParam = 3, 258, 3, 1.1515700
PPD_PropParam = 3, 258, 4, -1.9987300
PPD_PropParam = 3, 258, 5, -3.1300300
PPD_PropParam = 3, 258, 6, 170.00000
PPD_PropParam = 3, 258, 7, 425.20000

[### Interaction Parameters]
[### (Component i ID, Component j ID, Parameter Array, Array(I,J), Array(J,I))]

[### Phys Prop Calculator]

PPC_Z = 1, 0.0000000
PPC_Z = 2, 0.0000000
PPC_Z = 3, 0.0000000
PPC_Z = 4, 0.0000000
PPC_Z = 5, 0.0000000

PPC_FLOW = 1.0000000
PPC_P = 1.0132500
PPC_T_K = 0.0000000
PPC_H = 0.0000000
PPC_S = 0.0000000
PPC_VF = 0.0000000
PPC_VF = 0.0000000
PPC_Range_BL = 1.0000000
PPC_Range_BU = 10.0000000
PPC_Property = 1
PPC_ENV_T_Min_K = 0.0000000
PPC_ENV_T_Max_K = 150.00000
PPC_ENV_Num_P = 5
PPC_ENV_Num_Plot_Points = 40
PPC_ENV_P = 1, 1.0000000
PPC_ENV_P = 2, 2.0000000
PPC_ENV_P = 3, 4.0000000
PPC_ENV_P = 4, 8.0000000
PPC_ENV_P = 5, 16.0000000

```



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