ChemSep™ - Extracting Property Data to *Excel*

New with Release 6.6 (April 2010)

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We have extended the databank manager that comes with *ChemSep* so that it is possible to extract basic physical property data and send the results to *Excel*

1. **Creating an Extract Template**
2. **Selecting Compounds**
3. **Extracting the Data**
4. **Inserting an Empty Column**
5. **Complete List of Property Constants**
6. **Temperature dependent properties**

A few notes before we start the tutorial.

1. It is possible to create an unlimited number of different extract formats.
2. The file that defines the output format must begin with the word *Extract* and ends with *.def* and must be saved in the bin folder of *ChemSep*.
3. The export definition file is case sensitive.

1. Creating an Extract Template

The first step is to create an export template in a plain text file along the same lines as described above. An example is shown in column 2 of the table below.

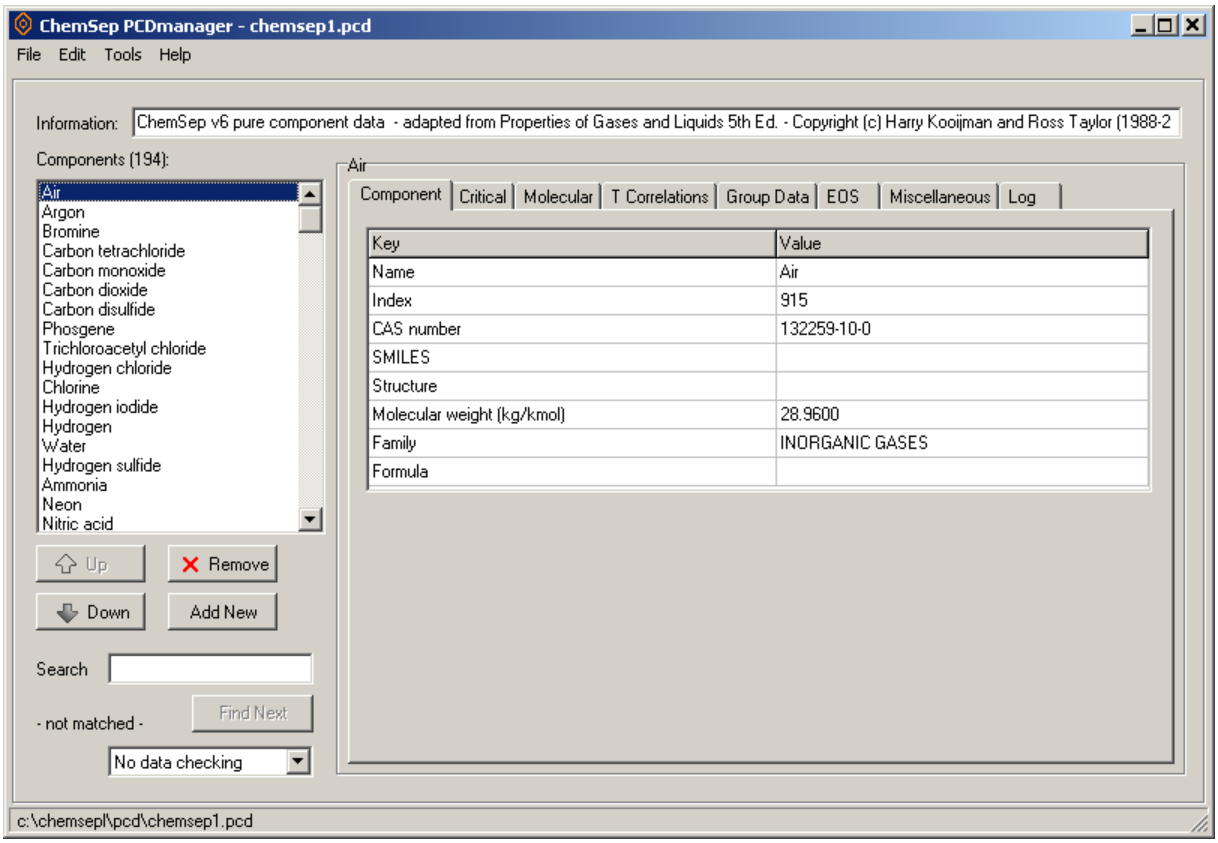
Line	Text	Meaning
1	**newsheet:**	Instruction to create a new worksheet (tab sheet)
2	Properties	Name of the worksheet (tab sheet) created by the instruction above
3	**var:**	Instruction to populate a new column on the worksheet named on line 2
4	Formula	Label that will appear on the top of the column (in row 3)
5		Line to enter the units to be used - empty because "Formula" has no units
6	Formula	Instruction to write the compound formula
7	**var:**	Instruction to populate a new column on the worksheet
8	Structure	Label that will appear on the top of the column (in row 3)
9		Units for the quantity to be displayed in this column
10	Structure	Instruction to write the compound structure
11	**var:**	Instruction to populate a new column on the worksheet
12	MW	Label that will appear on the top of the column (in row 3)
13	kg/kmol	Units for the quantity to be displayed in this column
14	Molecular weight	Instruction to write the compound molecular weight
15	**var:**	Instruction to populate a new column on the worksheet
16	SG	Label that will appear on the top of the column (in row 3)
17		Units for the quantity to be displayed in this column
18	Specific gravity	Instruction to write the compound specific gravity
19	**var:**	Instruction to populate a new column on the worksheet
20	Tboil	Label that will appear on the top of the column (in row 3)
21	C	Units for the quantity to be displayed in this column
22	Normal boiling point	Instruction to write the compound normal boiling point
23	**var:**	Instruction to populate a new column on the worksheet
24	Tmelt	Label that will appear on the top of the column (in row 3)
25	F	Units for the quantity to be displayed in this column
26	Melting point	Instruction to write the compound melting point

Save lines 1 to 26 of column 2 only to a text file. You may use any text editor – such as *Notepad*, but not *Word*, or *Wordpad* – for this purpose. The name of the file must begin with the word *Extract* and the extension must be *.def*. The rest of the name is up to you. The file must be saved in (or copied to) the bin folder of *ChemSep*.

Now start the properties databank management system (from the *Databanks* menu in *ChemSep*).

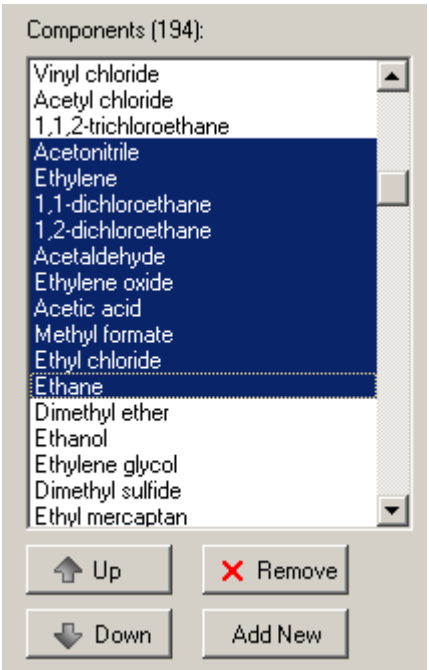
2. Selecting Compounds

When the databank manager starts you should see this:

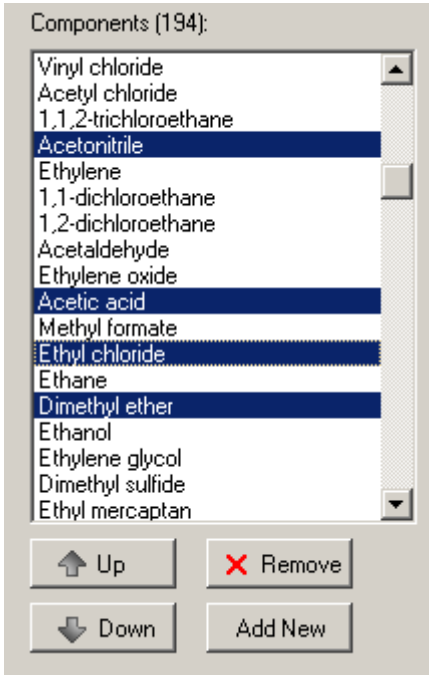


Next, to select the compounds whose data you wish to extract you must highlight the names of the desired compounds in the left hand panel using the mouse pointer. In the illustration above the only highlighted compound is air (the first one in the list on the left).

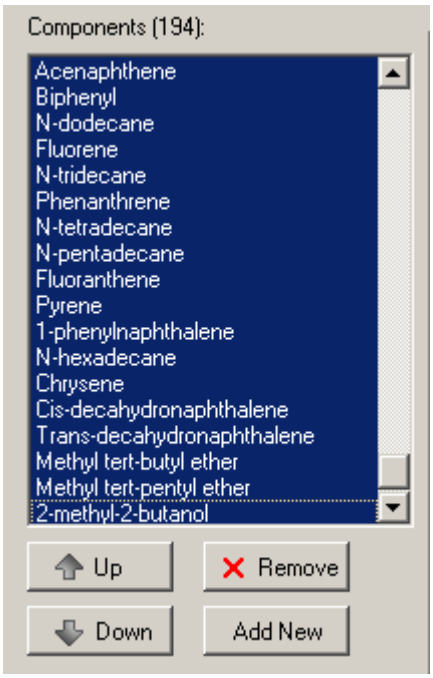
Hold down the *Shift* key while using the pointer to highlight a sequence of compounds:



Hold down the *Ctrl* key while using the pointer to highlight a non-contiguous set of compounds:



Hold down Ctrl-A to highlight all of the compounds in the databank.



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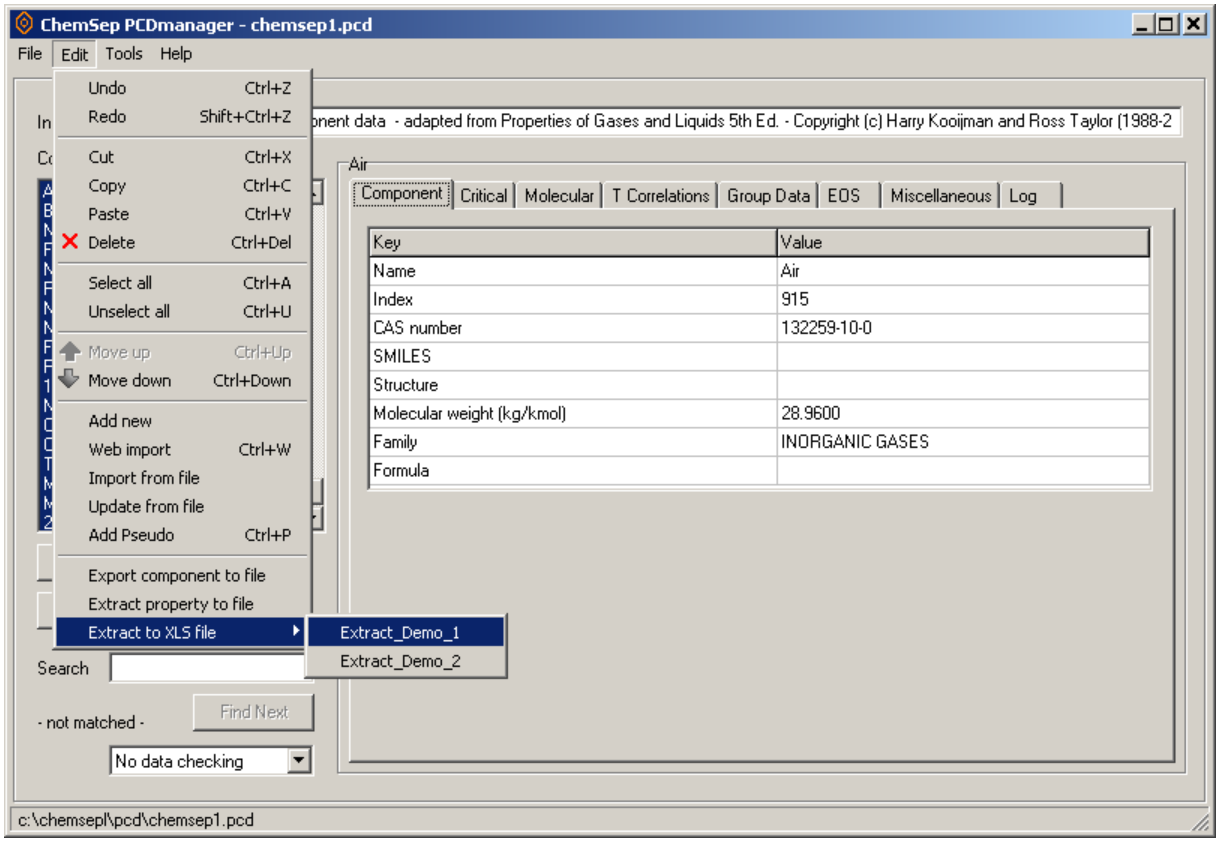
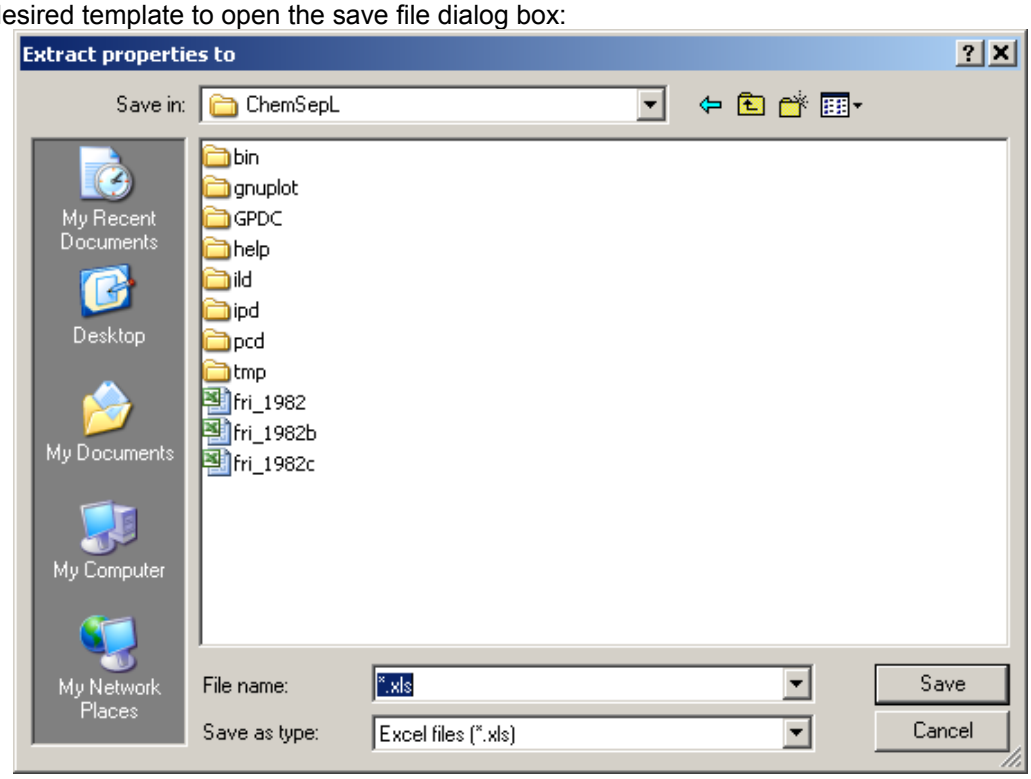
3. Extracting the Data

Now use the pointer to select *Edit* and then *Extract to Excel*. A list will appear of all the file names that have extract templates (i.e. that have names starting with *Extract* and ending with *.def*). In this case there are two such file: *Export_Demo_1.def* and *Export_Demo_2.def.*

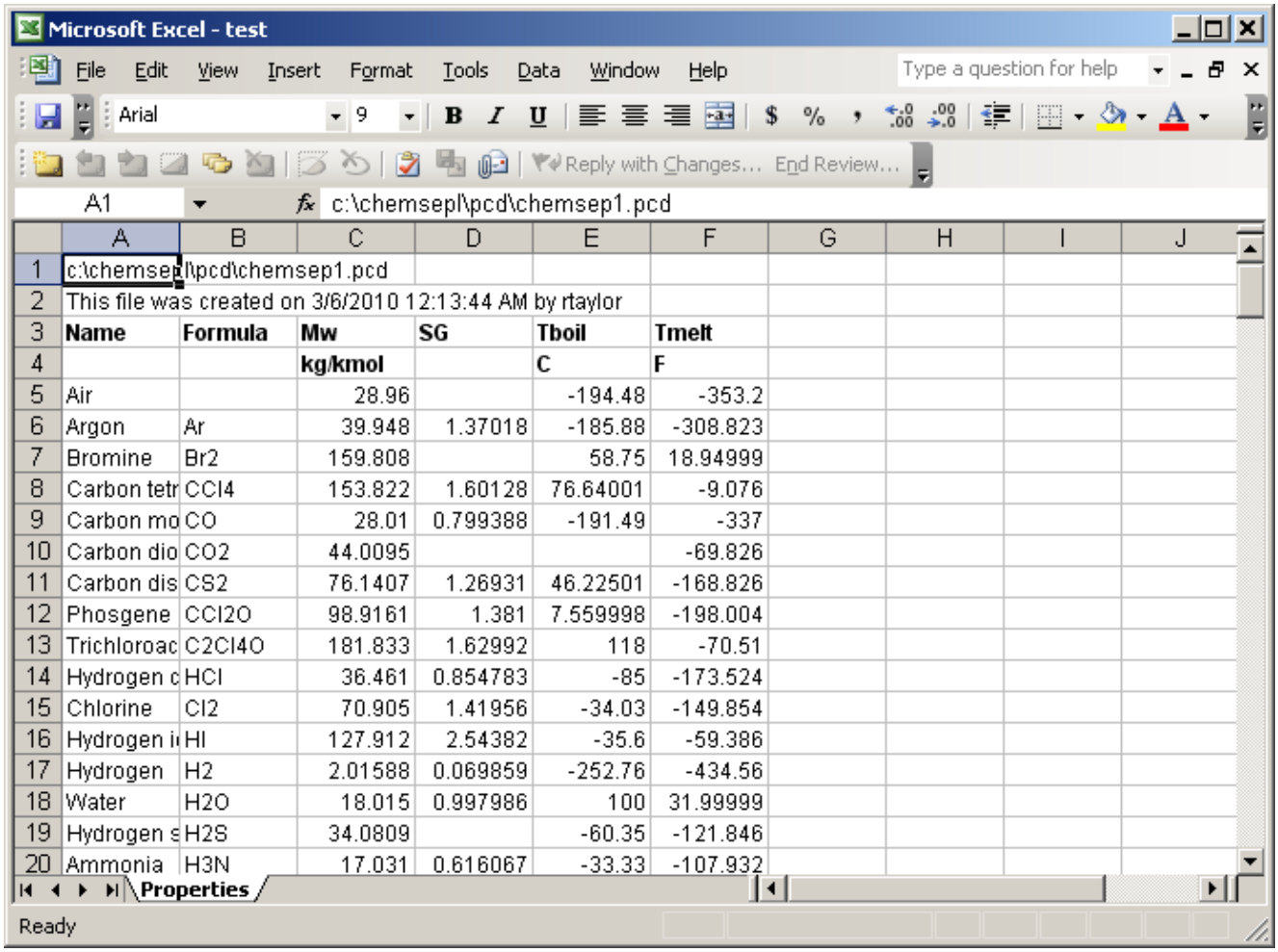


Select the desired template to open the save file dialog box:



Type in the desired name for the file and click *Save*.

Open the newly created Excel file to see the table that you have created.



	A	B	C	D	E	F	G	H	I	J
1	c:\chemsep1\pcd\chemsep1.pcd									
2	This file was created on 3/6/2010 12:13:44 AM by rtaylor									
3	**Name**	**Formula**	**Mw**	**SG**	**Tboil**	**Tmelt**				
4			**kg/kmol**		**C**	**F**				
5	Air		28.96		-194.48	-353.2				
6	Argon	Ar	39.948	1.37018	-185.88	-308.823				
7	Bromine	Br2	159.808		58.75	18.94999				
8	Carbon tetr	CCl4	153.822	1.60128	76.64001	-9.076				
9	Carbon mo	CO	28.01	0.799388	-191.49	-337				
10	Carbon dio	CO2	44.0095			-69.826				
11	Carbon dis	CS2	76.1407	1.26931	46.22501	-168.826				
12	Phosgene	CCl2O	98.9161	1.381	7.559998	-198.004				
13	Trichloroac	C2Cl4O	181.833	1.62992	118	-70.51				
14	Hydrogen c	HCl	36.461	0.854783	-85	-173.524				
15	Chlorine	Cl2	70.905	1.41956	-34.03	-149.854				
16	Hydrogen i	HI	127.912	2.54382	-35.6	-59.386				
17	Hydrogen	H2	2.01588	0.069859	-252.76	-434.56				
18	Water	H2O	18.015	0.997986	100	31.99999				
19	Hydrogen s	H2S	34.0809		-60.35	-121.846				
20	Ammonia	H3N	17.031	0.616067	-33.33	-107.932				

Properties

Ready

Exercise: Edit the .def file and change the units of the properties.

4: Inserting an Empty Column

How can you modify the above to create a spreadsheet with an empty column between the columns for temperature and pressure?

Given how the template is constructed (the four lines per variable) we can see that adding four lines (the first of which says *var:* and the remaining three being empty) should accomplish our goal (as long as we insert the four lines in the right place).

Exercise Edit the example created above to

5. Complete List of Property Constants

The template used to create this Excel file is just one example of what is possible. Any of the properties shown in the tables of PCDman can be exported using the key words and phrases in column 1 of the tale that appears below.

Property Name	Short Name (if any)	Default Units
Name		
Index		
CAS Number		
SMILES string		
Structure		
Molecular weight		kg/kmol
Family		
Critical temperature	Tc	K
Critical pressure	Pc	Pa
Critical volume		m^3
Critical compressibility factor		
Normal boiling point	Tnbp	K
Melting point	Tmelt	K
Triple point temperature	Ttp	K
Triple point pressure	Ppt	Pa
Liquid molar volume at normal boiling point		m^3/kmol
Acentric factor		
Radius of gyration		m
Solubility parameter		$(J/m^3)^{1/2}$
Dipole moment		Coulomb.m
Van der Waals volume		m^3
Van der Waals area		m^2
IG heat of formation		J/kmol
IG Gibbs energy of formation		J/kmol
IG absolute entropy		J/kmol.K
Heat of fusion at melting point		J/kmol
Heat of vaporization at normal boiling point		J/kmol
Standard net heat of combustion		J/kmol
COSTLD characteristic volume		m^3/kmol
Lennard Jones diameter		m
Lennard Jones energy		K
Rackett parameter		
Fuller et al. diffusion volume		
Surface tension at normal boiling point		N/m
Parachor		$kg^{1/4}m^3s^{1/2}kmol$

Property Name	Short Name (if any)	Default Units
Specific gravity		
SRK acentric factor		
Wilson volume		m^3/kmol
UNIQUAC r		
UNIQUAC q		
UNIQUAC q'		
API-SRK s1		
API-SRK s2		
Chao-Seader acentric factor		
Chao-Seader solubility parameter		$(J/m^3)^{1/2}$
Chao-Seader liquid volume		m^3/kmol

6. Exporting Temperature Dependent Properties

It is also possible to export pure component temperature dependent properties such as the vapor pressure, surface tension, and liquid density.

The basic format for exporting a temperature dependent property is:

```
var:
Title
Units
PropertyFunction(T)
```

The first three lines of this construction have the same function as in all other examples shown above. The fourth line includes the name of the function that evaluates the property and, in parentheses, the temperature at which the property is to be evaluated. For example, to evaluate the vapor pressure we can write:

```
VPC(300)

VPC(0.7*Tc)
```

The first of these two examples would evaluate the vapor pressure at a temperature of 300K, the second at a temperature equal to 70% of the critical temperature for that component. Other temperatures that are "known" to the temperature dependent property functions are

```
Tc          Critical temperature
Tmelt       Melting point
Tnbp        Normal boiling point
Ttp         Triple point temperature
```

The names of the temperature dependent property functions are tabulated below

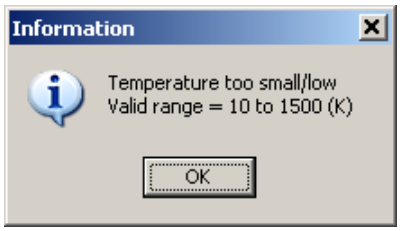
Property	Property Function	Default units
Vapor pressure	VPC	Pa
Solid density	SDNC	kmol/m^3
Liquid density	LDNC	kmol/m^3
Heat of vaporization	HVPC	J/kmol
Solid heat capacity	SCPC	J/kmol K
Ideal gas heat capacity	ICPC	J/kmol K
Liquid heat capacity	LCPC	J/kmol K
Second virial coefficient	SVRC	m^3/kmol
Liquid thermal conductivity	LTCC	W/m K
Vapor thermal conductivity	VTCC	W/m K
Antoine vapor pressure	ANTOINE	Pa
Surface tension	STC	N/m

The table below provides some more complete examples.

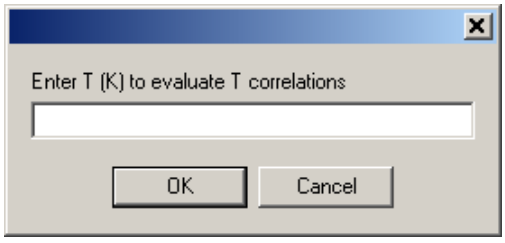
Line	Text	Meaning
1	**newsheet:**	Instruction to create a new worksheet (tab sheet)
2	Temperature dependent	Name of the worksheet (tab sheet) created by the instruction above
3	**var:**	Instruction to populate a new column on the worksheet named on line 2
4	Name	Label that will appear on the top of the column (in row 3)
5		Line to enter the units to be used - empty because "Name" has no units
6	Name	Instruction to write the compound name
7	**var:**	Instruction to populate a new column on the worksheet
8	Solid density at Tmelt	Label that will appear on the top of the column (in row 3)
9		Units for the quantity to be displayed in this column
10	SDNC(Tmelt)	Instruction to write the compound solid density at the compound melting point
11	**var:**	Instruction to populate a new column on the worksheet
12	Liquid density at Tmelt	Label that will appear on the top of the column (in row 3)
13		Units for the quantity to be displayed in this column
14	LDNC(Tmelt)	Instruction to write the compound liquid density at the compound melting point
15	**var:**	Instruction to populate a new column on the worksheet
16	Ideal gas Cp	Label that will appear on the top of the column (in row 3)
17		Units for the quantity to be displayed in this column
18	ICPC(380)	Instruction to write the compound ideal gas heat capacity
19	**var:**	Instruction to populate a new column on the worksheet
20	Liquid viscosity @ Tboil	Label that will appear on the top of the column (in row 3)
21		Units for the quantity to be displayed in this column
22	LVSC(Tboil)	Instruction to write the compound liquid viscosity at the boiling point
23	**var:**	Instruction to populate a new column on the worksheet
24	Antoine VP	Label that will appear on the top of the column (in row 3)
25	bar	Units for the quantity to be displayed in this column
26	ANTOINE(0.7 * Tc)	Instruction to write the compound vapor pressure from the Antoine equation

Save lines 1 to 26 of column 2 only to a text file. The name of the file must begin with the word *Extract*. The rest of the name is up to you. The file extension must be *.def* and the file must be saved in (or copied to) the bin folder of ChemSep.

A warning message is displayed in the event that the temperature specified falls outside the valid range for the correlation:



After clicking on OK you will be prompted for a temperature that can be used to evaluate the property:



Type in a number for the temperature and click OK..

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S
1	c:\chemse	2\pcd\chemsep1.pcd																	
2	This file was created on 4/8/2010 8:56:12 PM by rtaylor																		
3	Name	CAS Numb	Pvap@nbp	Pvap(0.7Tc)	Solid density	Liquid dens	Sublimatio	Vapor pres	Heat of vap	Solid heat	Liquid heat	Ideal gas h	Second viri	Liquid visc	Vapor visc	Liquid ther	Vapor ther	Surface ter	Surface ter
4		-	bar	bar	kmol/m3	kmol/m3	Pa	Pa	J/mol	J/mol/K	J/mol/K	J/mol/K	m3/kmol	Pa.s	Pa.s	W/m/K	W/m/K	N/m	N/m
5	Air	132259-10	1.02316891	3.824475		33.31876	6217.886	382447.5	5907.412		54.47254	28.89629		0.000173	6.55E-06	0.147934	0.008637		
6	Argon	7440-37-1	1.00926336	4.94564625		35.52753	6841.55	494564.6	6424.459		46.25857	20.78367	-0.10505	0.000262	8.64E-06	0.122844	0.005433	0.008075	0.008075
7	Bromine	7726-95-6	1.02403547	7.65211438		20.08899	6269.224	765211.4	29752.82	51.80269		35.78749	-0.17495	0.000709	2.07E-05	0.115601	0.007002	0.023212	0.023212
8	Carbon tetr	56-23-5	1.01292094	2.92850531	11.613019	10.85462	1104.754	292850.5	29719.27	93.16234	139.6123	88.52678	-0.598	0.000482	1.29E-05	0.091189	0.009839	0.01548	0.01548
9	Carbon mo	630-08-0	1.01549219	3.12096125	34.0360794	30.13694	15501.38	312096.1		40.89053	63.67327	29.02093	-0.13067	0.000169	6.21E-06	0.139987	0.008072	0.007145	0.007145
10	Carbon dio	124-38-9	67.302805		34.5851021	26.82767	5180075.9		4548.708	47.68944		37.05626	-0.11208	6.13E-05	1.07E-05	0.077532	0.010277		
11	Carbon dis	75-15-0	0.98281898	6.18721688	20.41009974	19.05351	0.675933	618721.7	26839.51	48.64343	78.01597	46.49159	-0.26089	0.000302	1.3E-05		0.012366	0.018621	0.018621
12	Phosgene	75-44-5	1.00601375	3.56847031		16.81866	1.920776	356847	24533.6	55.34514		56.19877	-0.2348	0.000549	9.96E-06	0.136195	0.009703	0.016101	0.016101
13	Trichloroac	76-02-8	1.04462469	2.34354203	10.7161961	9.573461	0.915812	234354.2	35302.94		177.2734	120.2605	-0.55571	0.000661	1.14E-05	0.097255	0.010052	0.018767	0.018767
14	Hydrogen c	7647-01-0	1.01007695	6.1837175	39.9247322	34.70002	13005.39	618371.8	16213.72	41.98844		29.08853	-0.09897	0.000349	1.12E-05		0.010695	0.018057	0.018057
15	Chlorine	7782-50-5	1.00619055	6.5492225		24.35163	1434.299	654922.3	20420.83	45.99968		32.69859	-0.17197	0.000484	1.32E-05	0.163832	0.008661	0.018258	0.018258
16	Hydrogen ii	10034-85-2	1.00941711	7.64745125		22.35863	494480.75	764745.1	20017.54	45.64127	59.12425	29.00338		0.001319	1.89E-05	0.051118	0.006112	0.017393	0.017393
17	Hydrogen	1333-74-0	1.00803813	2.15538672		38.39423	6969.297	215538.7	897.6861		20.43229		-0.09501	1.33E-05	1.27E-06	0.099858	0.018397	0.001485	0.001485
18	Water	7732-18-5	0.98036727	9.97339813	50.89591 98	56.47802	463.4485	997339.8	40744.93	26.60549	75.98555	34.2077	-0.03024	0.000278	1.55E-05	0.680947	0.031645	0.042197	0.042197
19	Hydrogen s	7783-06-4	0.99160352	7.28837625		29.07229	22106.24	728837.6	18736.53		68.74304	33.32571	-0.02932	0.000353	1.12E-05	0.232429	0.01186	0.015601	0.015601
20	Ammonia	7664-41-7	1.02208039	6.27606938	47.9729958	43.17217	6286.734	627606.9	23322.3	35.91719	77.89012	34.38082	-0.06291	0.000252	9.63E-06	0.613331	0.023317	0.023649	0.023649
21																			

The screen shot at left shows the Excel panel for many of the temperature dependent properties that resulted from using the *Extract_Demo_2.def* file with *ChemSep*.