

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	С	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).

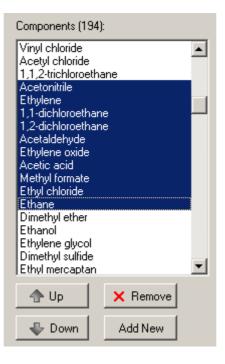
2. Selecting Compounds

When the databank manager starts you should see this:

ormation: ChemSep v6 pure compo	nent data - adapted from Properties of Gases and	Liquids 5th Ed Copyright (c) Harry Kooijman and Ross Taylor (1988-
mponents (194):	Air	
raon	Component Critical Molecular T Correl	ations Group Data EOS Miscellaneous Log
romine —	Key	Value
arbon tetrachloride arbon monoxide	Name	Air
arbon dioxide	Index	915
arbon disulfide hosgene	CAS number	132259-10-0
richloroacetyl chloride	SMILES	132203-10-0
ydrogen chloride		
hlorine ydrogen iodide	Structure	
ydrogen	Molecular weight (kg/kmol)	28.9600
ater	Family	INORGANIC GASES
ydrogen sulfide mmonia	Formula	
eon		
itric acid]	
슈 Up 🛛 🗙 Remove		
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arch		
Find Next		

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:

Components (194):						
Vinyl chloride Acetyl chloride 1,1,2-trichloroethane						
Acetonitrile						
Ethylene 1,1-dichloroethane 1,2-dichloroethane Acetaldehyde Ethylene oxide						
Acetic acid						
Methyl formate						
Ethyl chloride Ethane						
Dimethyl ether						
Ethanol						
Ethylene glycol Dimethyl sulfide Ethyl mercaptan	•					
🛧 Up 🗙 Remove						
🕹 Down 🛛 Add New						

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

Components (194):					
Acenaphthene Biphenyl N-dodecane Fluorene N-tridecane Phenanthrene N-tetradecane N-pentadecane Fluoranthene Pyrene 1-phenylnaphthale N-hexadecane Chrysene Cis-decahydronap Trans-decahydron	ohthalene haphthalene				
Methyl tert-butyl ether Methyl tert-pentyl ether 2-methyl-2-butanol					
🛧 Up 🗙 Remove					
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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*.

() C	🛇 ChemSep PCDmanager - chemsep1.pcd							
File	Edi	t Tools Help						
		Undo	Ctrl+Z					1
In	I	Redo Sh	hift+Ctrl+Z	pne	int da	ata - adapted from Properties of Gases and Liquids 5th Ec	d Copyright (c) Harry Kooijman and Ross Taylor (1988-2	
C	C	Cut	Ctrl+X		⊢Air			
4		Сору	Ctrl+C		(î)	Component Critical Molecular T Correlations Group	Data EOS Miscellaneous Log	
		Paste	Ctrl+V					
Ē	<u>×</u>	Delete	Ctrl+Del	_		Key	Value	
ĥ		Select all	Ctrl+A			Name Index	Air 915	
		Unselect all	Ctrl+U			CAS number	132259-10-0	
	+	Move up	Ctrl+Up			SMILES		
1	₽	Move down	Ctrl+Down			Structure		
		Add new				Molecular weight (kg/kmol)	28.9600	
		Web import	Ctrl+W			Family	INORGANIC GASES	
Ň		Import from file		Ы		Formula		
N 2		Update from file		H.				
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		Extract property						
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Select the desired template to open the save file dialog box:

Extract propertie	es to				<u>? ×</u>
Save in:	🛅 ChemSepL		•	🗢 🗈 💣 🎟	
My Recent Documents Desktop My Documents My Computer	bin GPDC help ild pcd fri_1982 fri_1982b fri_1982c				
My Network Places	File name: Save as type:	Excel files (*.xls)		•	Save Cancel

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.

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4	Name	ronnula	kg/kmol	30	C	F					-
5	Air		28.96		-194.48	-353.2					-
6		Ar	39.948	1.37018	-194.48	-308.823					-
7		Br2	159.808	1.37010	58.75	18.94999					-
8	Carbon tetr		153.822	1.60128	76.64001	-9.076					-
9	Carbon tet		28.01	0.799388	-191.49	-3.070					-
10	Carbon dio		44.0095	0.733300	-131.43	-69.826					-
11	Carbon dis		76.1407	1.26931	46.22501	-168.826					-
12	Phosgene		98.9161	1.381	7.559998	-198.004					-
13	Trichloroac		181.833	1.62992	118	-70.51					-
14	Hydrogen c		36.461	0.854783	-85	-173.524					-
15	· -	CI2	70.905	1.41956	-34.03	-149.854					
16	Hydrogen i	HI	127.912	2.54382	-35.6	-59.386					
17	· -	H2	2.01588	0.069859	-252.76	-434.56					
18		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					•
H A	H + > H Properties										
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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	Тс	К
Critical pressure	Pc	Pa
Critical volume		m ³
Critical compressibility factor		
Normal boiling point	Tnbp	К
Melting point	Tmelt	К
Triple point temperature	Ttp	К
Triple point pressure	Ppt	Pa
Liquid molar volume at normal boiling point		m³/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		m²
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		m³/kmol
Lennard Jones diameter		m
Lennard Jones energy		К
Rackett parameter		
Fuller et al. diffusion volume		
Surface tension at normal boiling point		N/m

Property Name	Short Name (if any)	Default Units
Specific gravity		
SRK acentric factor		
Wilson volume		m³/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		m³/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

Тс	Critical temperature
Tmelt	Melting point
Tnbp	Normal boiling point
Ttp	Triple point temperature

The names of the temperature dependent property functions are tabulated below

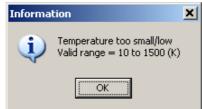
Property	Property Function	Default units
Vapor pressure	VPC	Pa
Solid density	SDNC	kmol/m ³
Liquid density	LDNC	kmol/m ³
Heat of vaporization	HVPC	J/kmol
Solid heat capacity	SCPC	J/kmol K
Ideal gas heat capacity	ICPC	J/kmol K
Liquid heat capacity	LCPC	J/kmol K
Second virial coefficient	SVRC	m ^{3.} /kmol
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:

	×
Enter T (K) to evaluate T correlations	
OK Cancel	

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

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3 Name	CAS Numb	Pvap@nbp	Pvap(0.7Tc)	CAS Numb Pvap@nbp Pvap(0.7Tc) Solid density Liquid dens Sublimatio/Vapor presHeat of vap Solid heat (Liquid heat Ideal gas h Second vir(Liquid visc/Vapor visc/Liquid ther/Vapor ther Surface tel Surface tel A	Liquid dens	Sublimatio	/apor pres	Heat of vap:	Solid heat (Liquid heat	Ideal gas h	Second viri	Liquid visc	Vapor visc	Liquid ther	Vapor theri	Surface tel	Surface te
4	-	bar	bar	kmol/m3	kmol/m3 F	Ра	Pa ,	J/mol	, Month	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	10	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	68641.55	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	Bromine 7726-95-6	1.02403547	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 te	Carbon tetr 56-23-5	1.01292094	1.01292094 2.92850531	1 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 m	Carbon mo 630-08-0	1.01549219	3.12096125	5 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 d	Carbon dio 124-38-9	67.302805		34.5851021	26.82767	518075.9		4548.708	47.68944		37.05626	-0.11208	6.13E-05	1.07E-05	0.077532	0.010277		
Carbon d	Carbon dis 75-15-0	0.98281898	6.18721688	8 20.4109974	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 Phosgen	Phosgene 75-44-5	1.00601375	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
3 Trichloro	Trichloroac 76-02-8	1.04462469	2.34354203	3 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	Hydrogen c 7647-01-0	1.01007695	6.1837175	5 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	Chlorine 7782-50-5	1.00619055	6.549225	5	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	Hydrogen ii 10034-85-2 1.00941711	1.00941711	7.64745125	5	22.35863	49480.75	764745.1	20017.54	45.64127	59.12425	29.00338		0.001319	1.89E-05	0.051118	0.006112	0.017393	0.017393
7 Hydroger	Hydrogen 1333-74-0	1.00803813	2.15538672	2	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	3 50.8959198	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	Hydrogen s 7783-06-4	0.99160352	7.28837625	5	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
	Ammonia 7664-41-7	1.02208039	6.27606938	8 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
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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*.