What's New in *ChemSep*™ 8.3

January 2022

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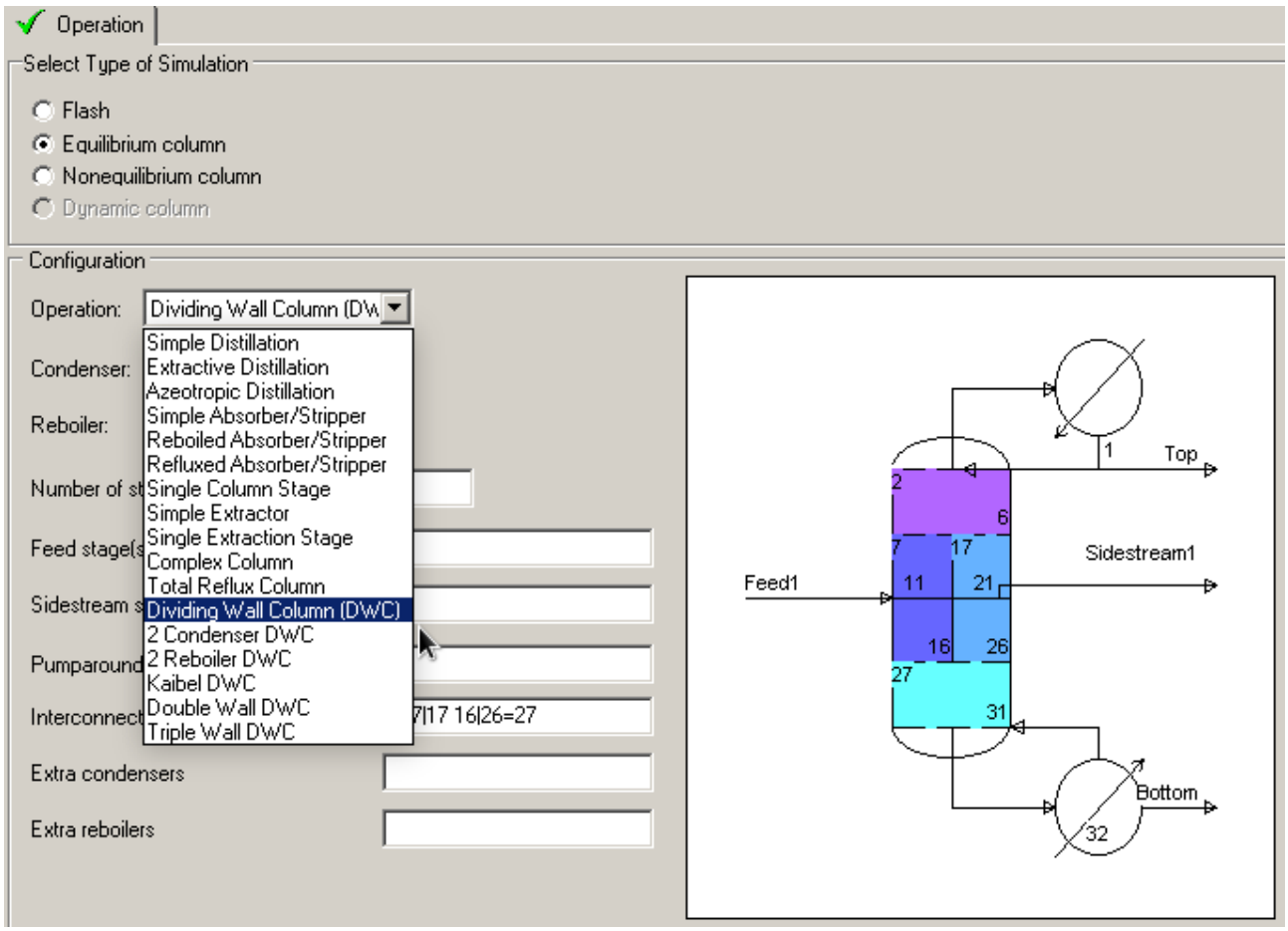
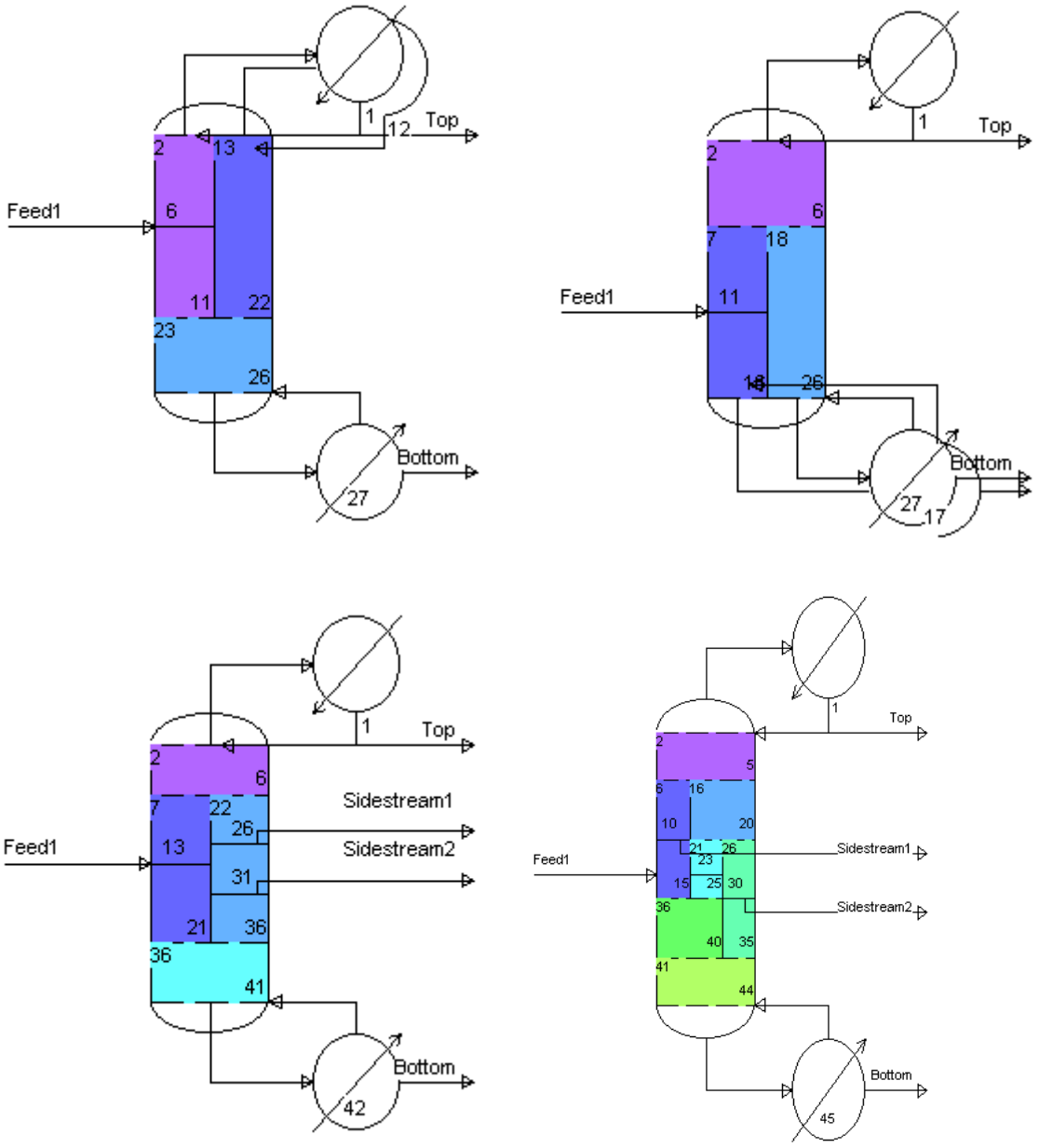
The following features were added:

- Fast set-up of Dividing Wall Columns (DWC) simulations
- Parity and Relative volatility diagrams for Vapor-Liquid Equilibria (VLE)
- New properties: Reid Vapor Pressure, Octane Number, and Total Vapor Pressure, ASTM D86 Temperatures
- New compounds and new tools in PCD manager

Fast Set-up of DWC Simulations

To facilitate a much quicker and easier set-up of DWC configurations, we added various column configurations with one, two, or three dividing walls and/or multiple condensers/reboilers. Default number of stages are assigned to each section but these can be adapted by left-clicking the various sections in the column drawing. This pops up an entry window to specify a new number of stages. Right-clicking allows adjustment of the cross-sectional area of the section as well as the fraction liquid flow to the section.



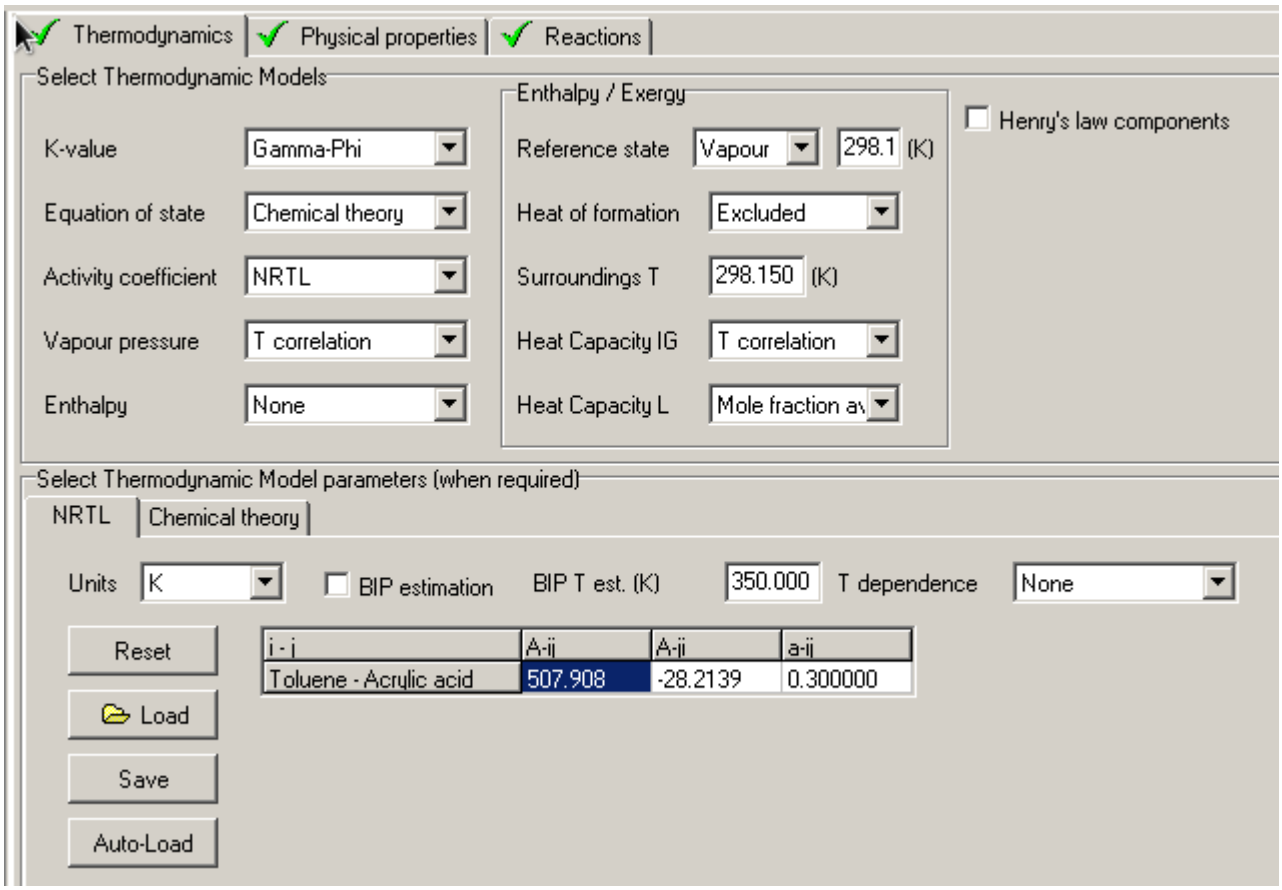


Vapor-Liquid Equilibria Parity & Relative Volatility Diagrams

To facilitate a quicker validation of VLE modeling, we added automated generation of relative volatility diagrams and creation of parity plots. To illustrate this, let us look at the VLE for Toluene / Acrylic Acid that we want to fit using the γ-φ model using NRTL for the liquid phase activity coefficients and chemical theory for the gas phase. First, enter the data in the comments field:

```
# Toluene - Acrylic Acid VLE data
ref=J.Chem.Eng.Data 56 pp. 3914-3939
url=https://pubs.acs.org/doi/pdf/10.1021/je200655s#
c1=108-88-3 Toluene
c2=79-10-7 Acrylic Acid
Txy@p=20kPa
335.25  1       1
336.44  0.859   0.934
336.78  0.826   0.923
336.95  0.773   0.906
337.87  0.721   0.886
339.3   0.637   0.859
340.3   0.564   0.819
340.59  0.53    0.814
341.39  0.484   0.781
343.32  0.406   0.75
344.02  0.378   0.732
345.44  0.321   0.676
348.05  0.249   0.611
349.77  0.215   0.575
352.72  0.171   0.492
356.29  0.121   0.388
361.67  0.057   0.209
365.82  0.025   0.108
368.4   0       0
```

Next, load the two components and setup the thermodynamic model:

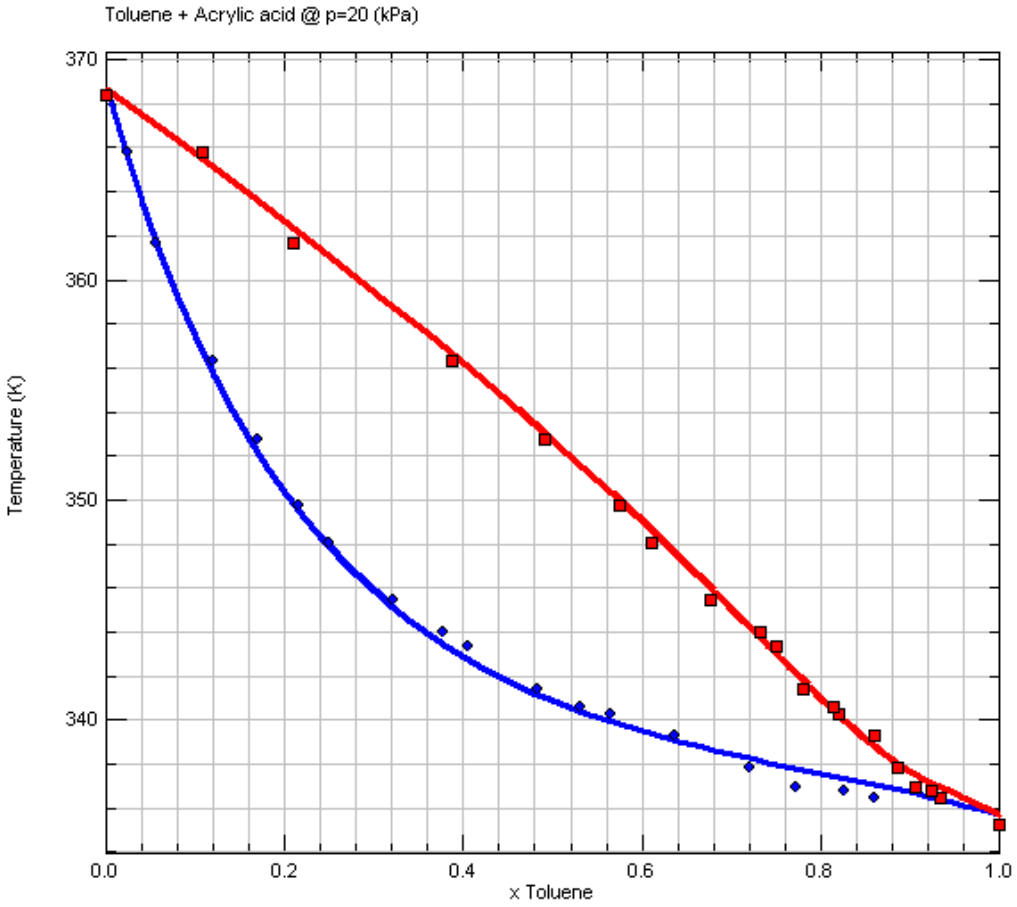


Under *Analysis*, select the Binary Phase Diagram option. Switch to the Data tab sheet and click on the file button. Since data is present in the comments field,

ChemSep will offer you the option to import that data from the comments. Select *yes* to import. The imported data will looks as follows:

```
Txy;
p=20kPa, T=335.25, x=1, y=1;
p=20kPa, T=336.44, x=0.859, y=0.934;
p=20kPa, T=336.78, x=0.826, y=0.923;
p=20kPa, T=336.95, x=0.773, y=0.906;
p=20kPa, T=337.87, x=0.721, y=0.886;
p=20kPa, T=339.3, x=0.637, y=0.859;
p=20kPa, T=340.3, x=0.564, y=0.819;
p=20kPa, T=340.59, x=0.53, y=0.814;
p=20kPa, T=341.39, x=0.484, y=0.781;
p=20kPa, T=343.32, x=0.406, y=0.75;
p=20kPa, T=344.02, x=0.378, y=0.732;
p=20kPa, T=345.44, x=0.321, y=0.676;
p=20kPa, T=348.05, x=0.249, y=0.611;
p=20kPa, T=349.77, x=0.215, y=0.575;
p=20kPa, T=352.72, x=0.171, y=0.492;
p=20kPa, T=356.29, x=0.121, y=0.388;
p=20kPa, T=361.67, x=0.057, y=0.209;
p=20kPa, T=365.82, x=0.025, y=0.108;
p=20kPa, T=368.4, x=0, y=0;
```

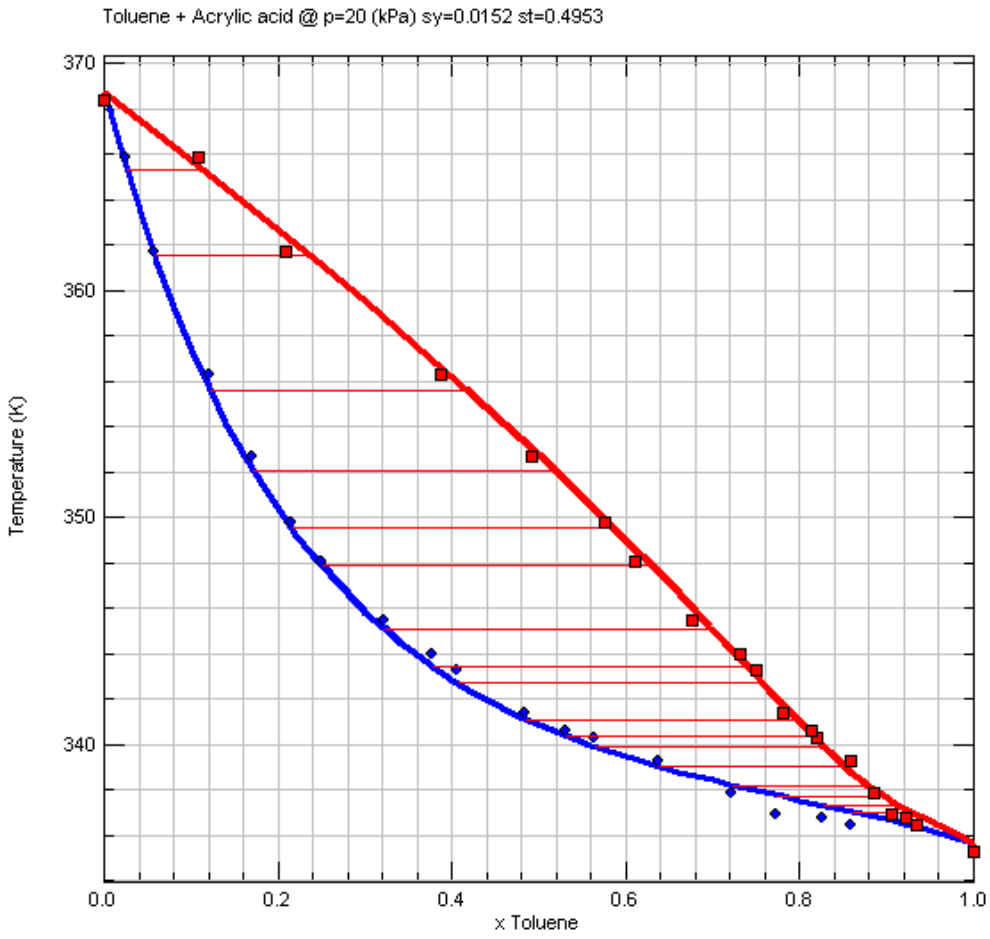
Click on the Calculate tab to create the phase diagram; click on the *Plot* tab to display it.



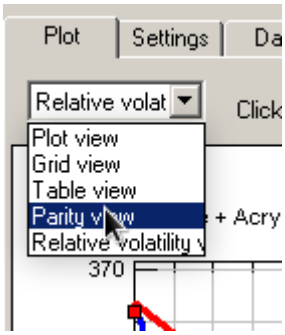
Using the △ Data button, we now can generate the *y* and *T* computed from the measured liquid compositions *x* and pressure *p* that appear on the data tab:

Txy;
p=20kPa, T=335.25, x=1, y=1;
p=20kPa, T=336.44, x=0.859, y=0.934,u=337.0165,z=0.927999;
p=20kPa, T=336.78, x=0.826, y=0.923,u=337.2949,z=0.914551;
p=20kPa, T=336.95, x=0.773, y=0.906,u=337.7405,z=0.895347;
p=20kPa, T=337.87, x=0.721, y=0.886,u=338.1921,z=0.878374;
p=20kPa, T=339.3, x=0.637, y=0.859,u=339.0097,z=0.851938;
p=20kPa, T=340.3, x=0.564, y=0.819,u=339.878,z=0.827678;
p=20kPa, T=340.59, x=0.53, y=0.814,u=340.3575,z=0.815042;
p=20kPa, T=341.39, x=0.484, y=0.781,u=341.1022,z=0.796085;
p=20kPa, T=343.32, x=0.406, y=0.75,u=342.7009,z=0.756746;
p=20kPa, T=344.02, x=0.378, y=0.732,u=343.4006,z=0.739715;
p=20kPa, T=345.44, x=0.321, y=0.676,u=345.0939,z=0.696938;
p=20kPa, T=348.05, x=0.249, y=0.611,u=347.8907,z=0.628108;
p=20kPa, T=349.77, x=0.215, y=0.575,u=349.5313,z=0.58538;
p=20kPa, T=352.72, x=0.171, y=0.492,u=352.0547,z=0.517113;
p=20kPa, T=356.29, x=0.121, y=0.388,u=355.5819,z=0.416655;
p=20kPa, T=361.67, x=0.057, y=0.209,u=361.5343,z=0.234314;
p=20kPa, T=365.82, x=0.025, y=0.108,u=365.3015,z=0.112201;
p=20kPa, T=368.4, x=0, y=0;

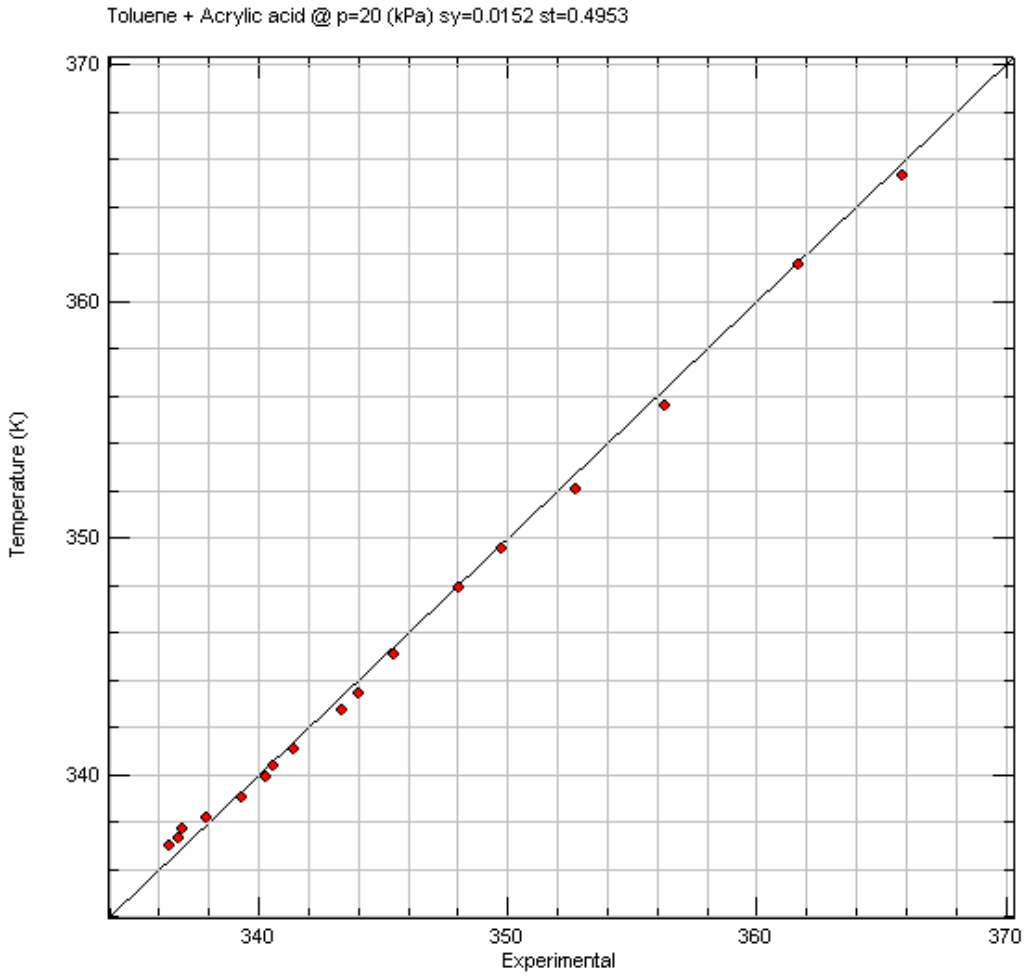
These pairs of points (*Tx* and *Ty*) are joined by horizontal lines on the binary phase diagram.



Go to the view selector in the top left corner of the plot window and choose the *Parity view* (this view selector also allows you to switch between text grids or table views with the data and computed values:



The parity plot now looks as follows:



To search if there are other VLE data sets published in literature for this mixture click the NIST button on the data panel. This opens the web-site of the National Institute for Standards and Technology in your default browser and enters the selected compounds:

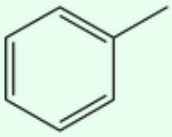
Home | Scope | Property | Report Draft | Compound Cache | Help | About

Measurement System & Property Selection

Select System Type: Help

Binary mixture

Name: toluene
Formula: C_7H_8
Other Names: methylbenzene
benzene, methyl-

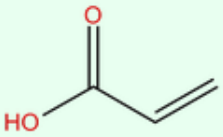


Help

New Compound Search

WTT Pro (subscription) / NIST Chemistry WebBook

Name: propenoic acid
Formula: $C_3H_4O_2$
Other Names: vinylformic acid
acrylic acid



Help

New Compound Search

WTT Pro (subscription) / NIST Chemistry WebBook

Select Property:

Help

Property Group: Vapor-liquid equilibria & solubility

Property: Vapor-liquid equilbria

Add result to Report Draft

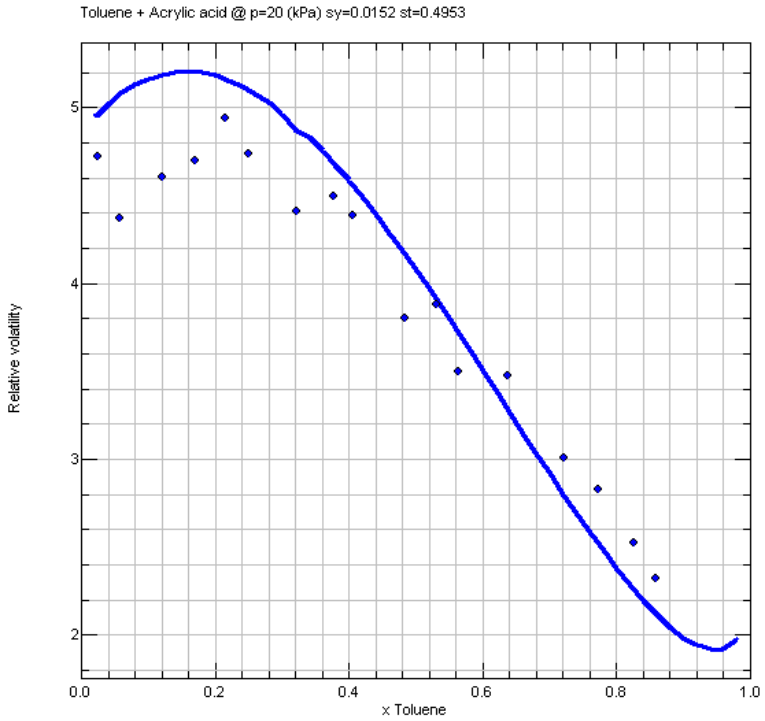
Compounds: propenoic acid
toluene
Measurement: Vapor-liquid equilbria

1 data source is listed in the NIST SOURCE Data Archive.

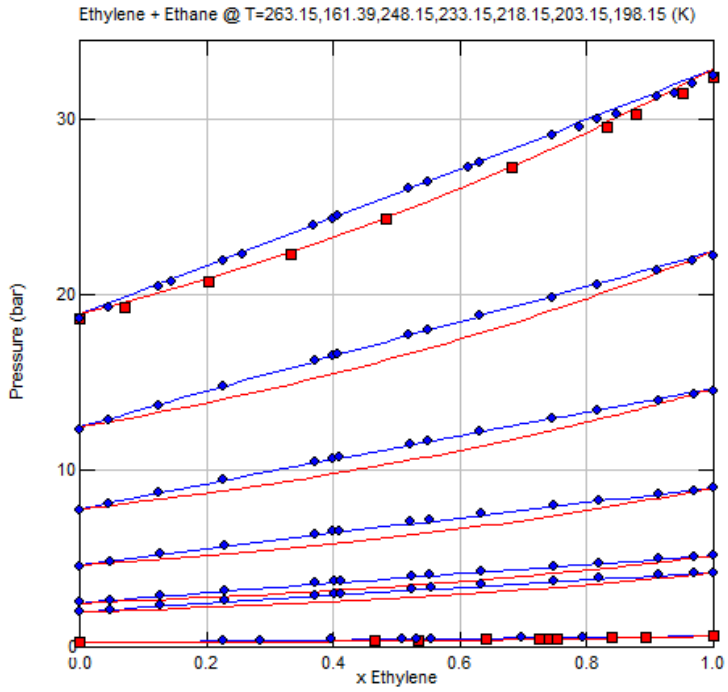
1. Huang, G.; Yao, S.; Zhao, Y.; Liu, L.
   Isobaric Vapor Liquid Equilibrium for Binary Systems of Toluene + Acrylic Acid, Toluene + Acetic Acid, and Cyclohexane + Acrylic Acid at 20 kPa
   J. Chem. Eng. Data, 2011, 56, 3914-3919
   Temperature: 335.25 K - 368.4 K
   Pressure: 20 kPa

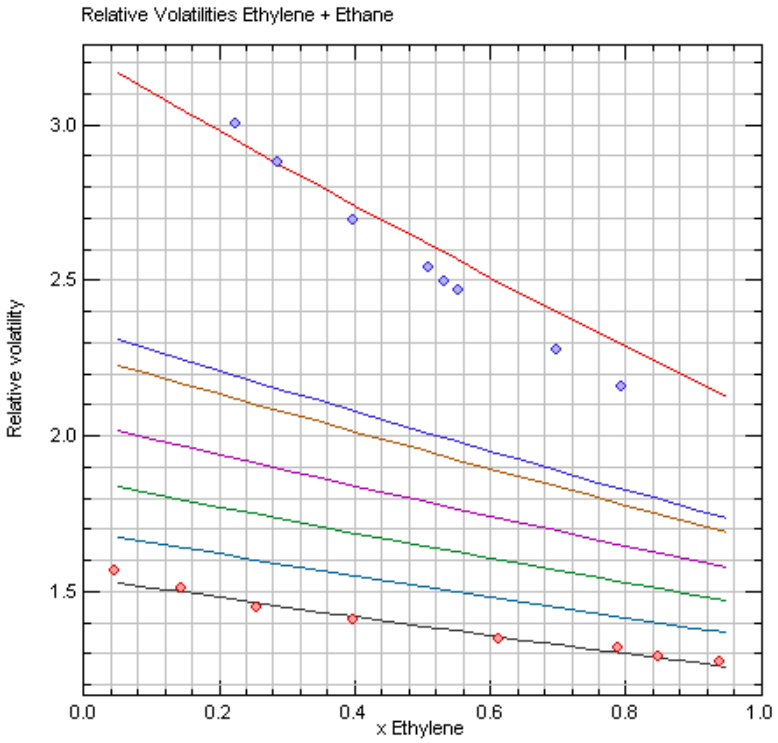
You will find out that this is the only citation for this specific mixture!

We can also choose the relative volatility plot which looks like:



You can see that at high Acrylic Acid mole fractions, the relative volatility has a maximum whereas at high Toluene composition it has a minimum.
It is also possible to display multiple sets of data on the phase diagram as well as on the parity plots, thereby making very easy a comparison of data and the model to verify that the selected model sufficiently well describes the VLE. Below is an example for the Ethylene and Ethane binary:





In case you are wondering why there are only two sets of relative volatility data when we see seven sets of VLE data, it is because only two of the data sets are complete sets of *pxy* data. The others are *px* data sets which don't allow the computation of relative volatilities (neither from *py* data).

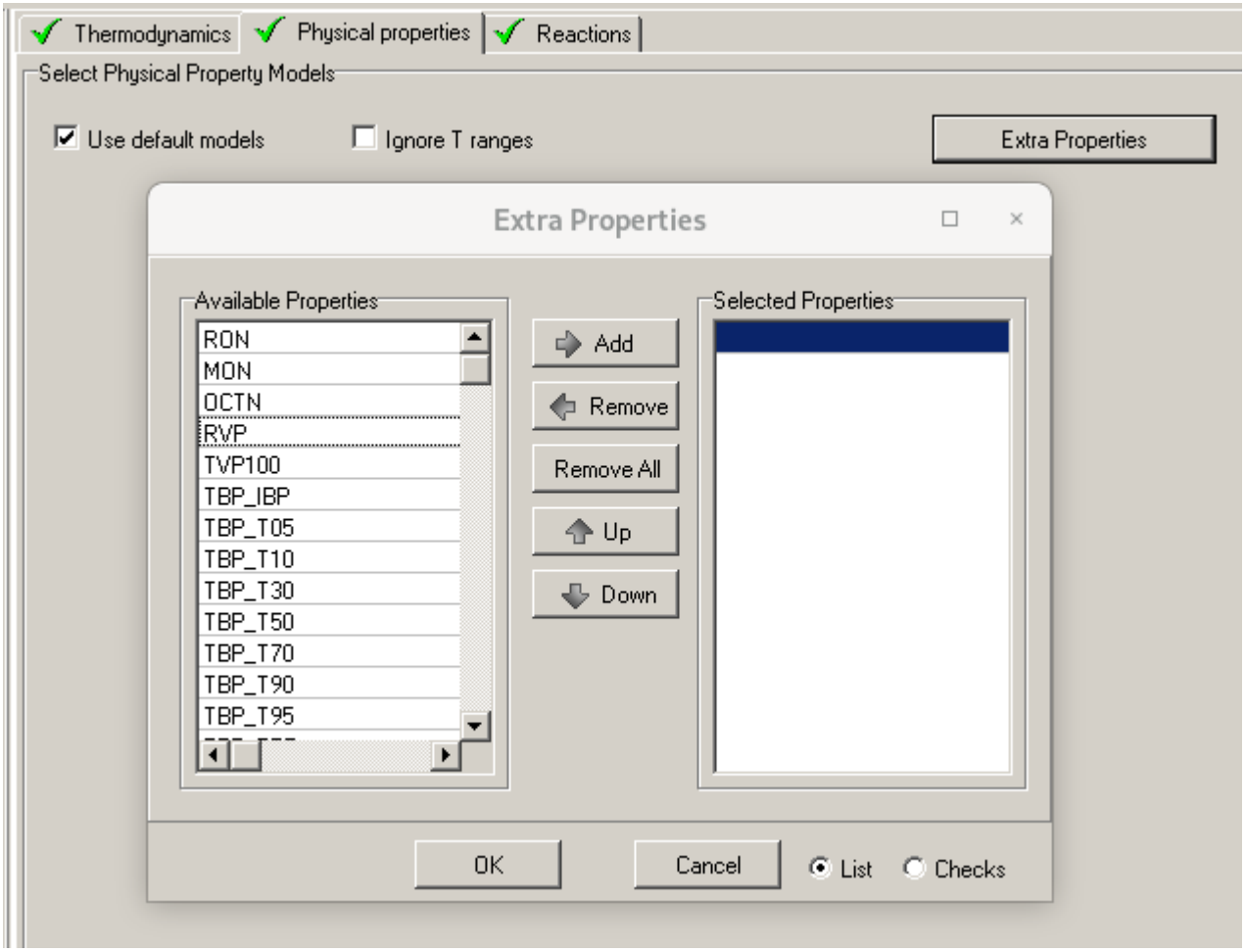
Extra Properties

For petrochemical process plants the following "petroleum properties" are often very useful:

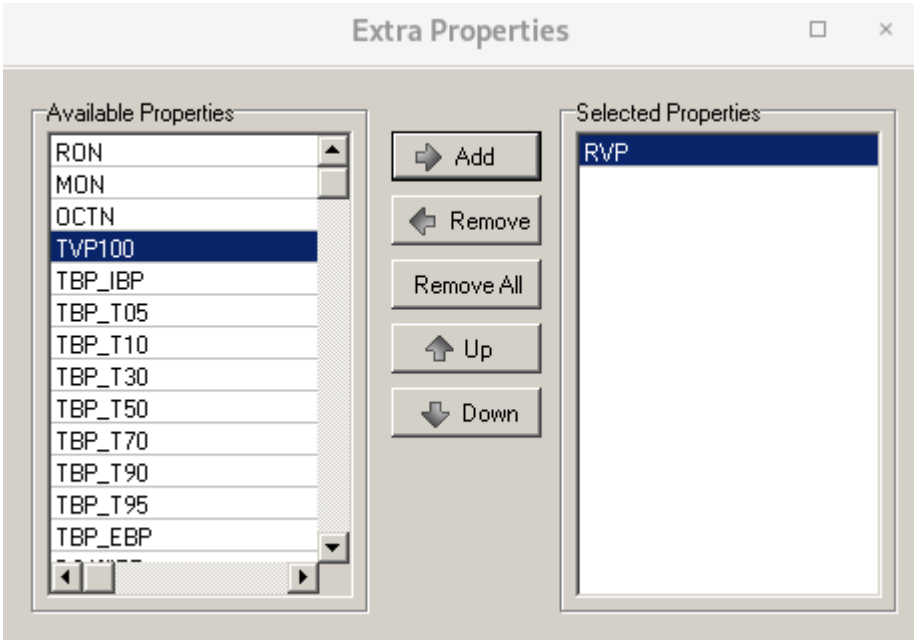
- RVP = Reid Vapor Pressure (in Pascal)
- TVP100 = Total Vapor Pressure at 100 F (in Pascal)
- MON = Motor Octane Number
- RON = Research Octane Number
- OCTN = Octane Number = (MON + RON) / 2
- D86_TXX = ASTM D86 temperature (in K) where XX is 05/10/30/50/70/90/95
- D86_IBP = ASTM D86 Initial Boiling Point temperature (in K)
- D86_EBP = ASTM D86 End Boiling Point temperature (in K)
- TBP_TXX = True Boiling Point temperatures (in K)
- FLASHPT = Flash point temperature (in K)

Note that the unit conversion is not yet available for these extra properties.

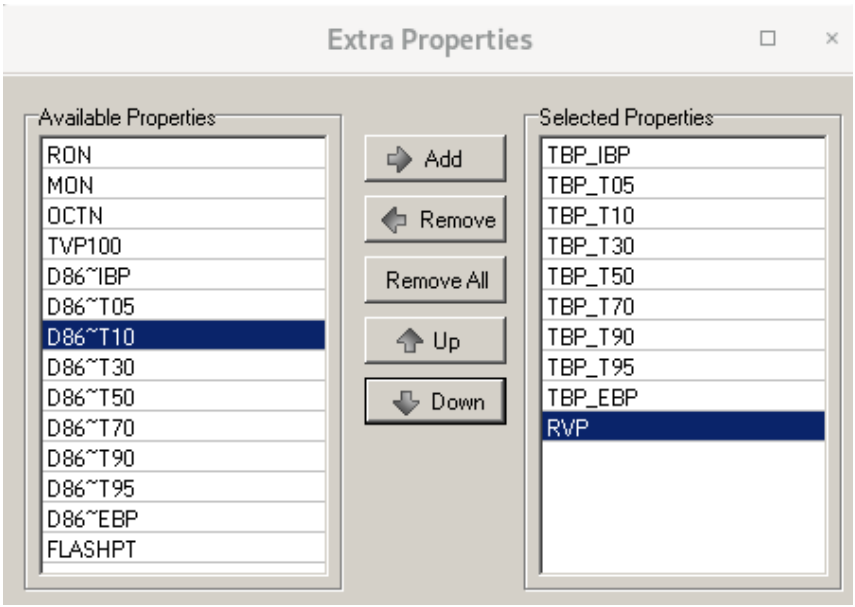
You can now compute this in ChemSep by selecting the extra properties under the physical properties:



Click the add to select the desired properties:



Note that you may select more than one property and add them in one go. In order to manipulate the output lines you can move the properties up or down to get the order that you so desire:



The output looks like this:

Stream	Feed1	Top	Bottom
Stage	20	1	25
Pressure (kPa)	101.325	101.325	101.325
Vapour fraction (-)	0.000000	0.000000	0.000000
Temperature (K)	389.036	383.619	413.557
Enthalpy (J/kmol)	-2.025E+07	-2.292E+07	-1.774E+07
Entropy (J/kmol/K)	-48804.1	-48611.2	-53766.8
Total molar flow (kmol/s)	2.00000	1.00000	1.00000
Total mass flow (kg/s)	164.201	91.9930	72.2080
Vapour std.vol.flow (m3/s)			
Liquid std.vol.flow (m3/s)	0.174092	0.105683	0.0684085
Liquid:			
Mole weight (kg/kmol)	82.1005	91.9934	72.2077
Density (kg/m3)	841.666	781.593	900.334
Std.density (kg/m3)	943.186	870.459	1055.54
Viscosity (N/m2.s)	2.7220E-04	2.3675E-04	2.8748E-04
Heat capacity (J/kmol/K)	176229	183750	161155
Thermal cond. (J/s/m/K)	0.120055	0.109780	0.124628
Surface tension (N/m)	0.0192383	0.0181556	0.0188929
Extra:			
TBP IBP	380.375	380.744	383.973
TBP T05	381.893	382.098	385.329
TBP T10	383.790	383.790	387.024
TBP T30	391.380	390.558	393.806
TBP T50	398.970	397.326	400.587
TBP T70	406.560	404.094	407.369
TBP T90	414.150	410.862	414.150
TBP T95	416.047	412.554	415.845
TBP EBP	417.565	413.907	417.202
RVP	4588.77	6712.39	1017

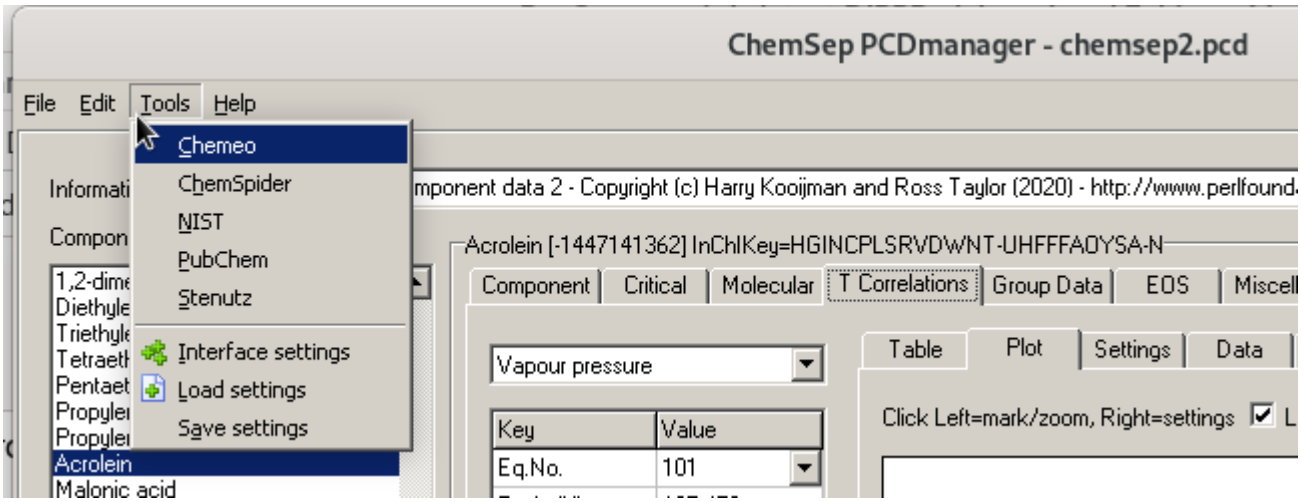
Miscellaneous Updates

Version 8.3 also includes many small improvements such as:

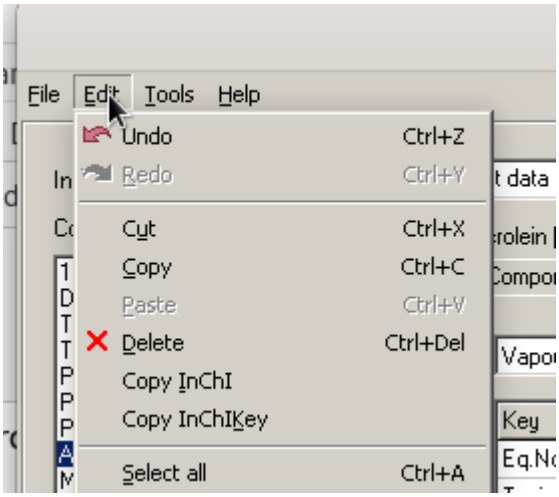
- Improved Antoine parameters of various components
- Added variables to the parametric study feature
- Bug fixes for the calculation of entropy production rates
- Improvements to some Group Contribution Methods
- Fixes to erroneous Parachor values of certain pure components
- New methods to estimate the Parachor

New Compounds and New Tools in PCD manager

Our Pure Component Data manager has additional options to get properties from several online databases such as Chemeo, ChemSpider, NIST, PubChem and others on the selected compound:



For this lookup to work you must have filled in a CAS number, name, or formula. We also enabled PCDmananger to show InChI and InChIKey. These are very useful in searching the internet and can be clipped to the clipboard via special options in the edit menu:



We added new components to our library, particularly fatty acids and their methyl esters as well as their glycerides for bio-fuel related simulations. They are available in ChemSep2.pcd which will be automatically searched when you select the wild card *.pcd in the search box of ChemSep. The following compounds reside in the new file:

57-55-6	1,2-propylene glycol
872-05-9	1-decene
112-41-4	1-dodecene
1120-36-1	1-tetradecene
629-73-2	1-hexadecene
112-88-9	1-octadecene
3452-07-1	1-eicosene
80-05-7	Bisphenol a
4286-23-1	P-isopropenyl phenol
2980-71-4	2-methyl-1-nonene
18516-37-5	2-methyl-1-undecene
18094-01-4	2-methyl-1-tridecene
29833-69-0	2-methyl-1-pentadecene
42764-74-9	2-methyl-1-heptadecene
52254-50-9	2-methyl-1-nonadecene
93-89-0	Ethyl benzoate
119-36-8	Methyl salicylate
122-79-2	Phenyl acetate
75-31-0	Isopropylamine
103-73-1	Phenetole
463-57-0	Methane-diol
4433-56-1	Ethane-1,1-diol
110-80-5	2-ethoxyethanol
107-07-3	2-chloroethanol
112-36-7	Diethylene glycol diethyl ether
7439-97-6	Mercury
101-84-8	Diphenyl ether
14371-10-9	t-Cinnamaldehyde
140-10-3	t-Cinnamic acid
122-97-4	3-phenyl-1-propanol
100-52-7	Benzaldehyde
100-51-6	Benzyl alcohol
65-85-0	Benzoic acid
94-36-0	Benzoyl peroxide
4780-79-4	1-Naphthalenemethanol
526-75-0	2,3-xylenol
105-67-9	2,4-xylenol
95-87-4	2,5-xylenol
576-26-1	2,6-xylenol
95-65-8	3,4-xylenol
108-68-9	3,5-xylenol
527-60-6	Mesitol
599-64-4	P-cumylphenol
837-08-1	O,p-bisphenol a
7722-84-1	Hydrogen peroxide
80-15-9	Cumene hydroperoxide
80-43-3	Dicumyl peroxide
98-49-7	P-diisopropylbenzene hydroperoxide
3071-32-7	Ethylbenzene hydroperoxide
110-71-4	1,2-dimethoxyethane
111-96-6	Diethylene glycol dimethyl ether
112-49-2	Triethylene glycol dimethyl ether
143-24-8	Tetraethylene glycol dimethyl ether
1191-87-3	Pentaethylene glycol dimethyl ether
107-98-2	Propylene glycol monomethyl ether
108-65-6	Propylene glycol monomethyl ether acetate
107-02-8	Acrolein

141-82-2	Malonic acid
108-59-8	Dimethylmalonate
53716-82-8	Cyrene
4792-15-8	PentaEthylene Glycol
2615-15-8	HexaEthylene Glycol
110-98-5	DiPropylene Glycol
1638-16-0	TriPropylene Glycol
24800-25-7	TetraPropylene Glycol
21482-12-2	PentaPropylene Glycol
-	HexaPropylene Glycol
64-18-6	Formic acid
142-62-1	Caproic acid
124-07-2	Caprylic acid
334-48-5	Capric acid
143-07-7	Lauric acid
544-63-8	Myristic acid
57-10-3	Palmitic acid
57-11-4	Stearic acid
112-80-1	Oleic acid
60-33-3	Linoleic acid
463-40-1	Linolenic acid
106-70-7	Methyl caproate
111-11-5	Methyl caprylate
110-42-9	Methyl caprate
111-82-0	Methyl laurate
124-10-7	Methyl myristate
112-39-0	Methyl palmitate
112-61-8	Methyl stearate
112-62-9	Methyl oleate
112-63-0	Methyl linoleate
301-00-8	Methyl linolenate
111-87-5	1-octanol
143-08-8	1-nonanol
112-30-1	1-decanol
112-42-5	1-undecanol
112-53-8	1-dodecanol
112-70-9	1-tridecanol
112-72-1	1-tetradecanol
629-76-5	1-pentadecanol
36653-82-4	1-hexadecanol
1454-85-9	1-heptadecanol
112-92-5	1-octadecanol
1454-84-8	1-nonadecanol
629-96-9	1-eicosanol
124-13-0	Octanal
124-19-6	Nonanal
112-31-2	Decanal
112-44-7	Undecanal
112-54-9	Dodecanal
10486-19-8	Tridecanal
124-25-4	Tetradecanal
2765-11-9	Pentadecanal
629-80-1	Hexadecanal
629-90-3	Heptadecanal
638-66-4	Octadecanal
17352-32-8	Nonadecanal
538-23-8	Tricaprylin
621-71-6	Tricaprin
538-24-9	Trilaurin
555-45-3	Trimyristin
555-44-2	Tripalmitin
555-43-1	Tristearin
122-32-7	Triolein
537-40-6	Trilinolein
14465-68-0	Trilenollenin
872-50-4	NMP