Getting started with Simulis[®] Thermodynamics

Use Case 5: Create pseudo-compounds from TBP and API gravity data curves

Software & Services In Process Simulation



We guide You to efficiency

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About pseudo-compounds.....

Simulis[®] Thermodynamics oil characterization environment enables you to characterize petroleum fluids using experimental data.

The oil will be characterized by a set of pseudo-compounds (or pseudo-components) in order to reduce the computational effort.

Each pseudo-compound will be defined by physical properties just like usual compounds. These properties are automatically generated from experimental data and used in the fluid thermodynamic package.

This document presents the different steps to follow in order to generate pseudo-compounds from a crude oil TBP 760 curve and an API gravity data curve.

The following steps will be followed:

- Step 1: Select the light ends (when necessary)
- Step 2: Enter assay characterization data
- Step 3: Generate the pseudo-compounds
- Step 4: Analyze the results

About pseudo-compounds.....

Method 1:

A petroleum cut can be characterized by selecting two or three of the following _____ properties:

- Normal boiling point.
- Molecular weight.
- Watson characterization factor.
- API degree.
- Specific gravity .

Method 2:

It can also be characterized by experimental distillation curve and gravity (or density) — data (TBP or ASTM curves).

PETROLEUM CUT	Use this window to create pseu	ido-compounds for a petroleum cut.
FILE	Select 2 or 3 known parameters	
Save as	Normal boiling point	
DATA	Molecular weight	
Paste data from clipboard	Watson characterization fa	ctor
Insert a new line	API Degree	
😈 Delete the current line	Specific gravity	
UNITS	▲ Data	
Molecular weight g/mol		
	Select the models used to calcul	ate the properties
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About pseudo-compounds...

All physical properties are calculated from an internally generated TBP curve at atmospheric conditions. All other curves are automatically converted into TBP curve.

Access the different types of curve.

Assay characterization		
Select the source curve type:	ASTM D1160 at 10 mmHg	~
	ASTM D1160 at 10 mmHg ASTM D1160 at 760 mmHg	_
Cor; data to clipboard	ASTM D1160 at P ASTM D2887 (Simulated Distillation) ASTM D86	
Paste data from clipboa	ASTM D86 corrected Simulation data	
Insert a new line	TBP at 10 mmHg	¥
Delete the current line		
🖄 Draw graph		
OPTIONS		
Mean API gravity		
No curve		
UNITS		
Temperature <mark>K</mark>		
Pressure Pa		
Options Light ends		onvert > Cancel

Preparation of the data

Prepare the required information in an Excel spreadsheet.

1. TBP distillation curve.

TBP dis	tillation
LV percent	°F
3.83	98
5	125
10	167
20	227
30	291
40	370
50	460
60	552
70	643
80	799
90	1023
100	1440

Light Ends, LV F	Percent on Crude
Propane	0.18
i-Butane	0.3
n-Butane	0.69

3. Light ends list and volume % on crude (if any light ends are identified).

API gravity					
Mid LV percent	°API				
12	66.7				
19	55.3				
40	37.6				
62	27				
82	19				

Mean API gravity

2. API gravity curve.

TBPCUTS :							
Tstart	Tend	Nb pseudos					
50	150	4					
150	550	16					
550	750	4					
750	1250	5					

35

4. Number of required pseudocompounds (optional).

Step 1: Select the light ends

ACCESS THE THERMODYNAMIC CALCULATOR EDITOR:

If you are using Simulis Thermodynamics in Excel:					
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		Simulis Compound			
	4	Simulis Compounds	rsonn	alisées	
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 If you are using Simulis Thermodynamics within another ProSim environnement (ProSimPlus, BatchReactor, BatchColumn etc...):

Click on the thermodynamic icon to open the calculator editor:



AB

Simulis Thermodynamics is a

 software component » that you can integrate into different applications:
 ProSim software, Excel, Matlab, your own software, etc...

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Step 1: Select the light ends



database and close the window.

Step 1: Select the light ends





- 1. Select a type of curve ("*TBP at 760* ~ *mmHg*" in this example).
- 2. Select your options for defining the _____ gravity.
- 3. Select your temperature unit ("°F' in this example).



Enter your experimental values for the TBP and the API gravity.

- -22 Assay characterization Select the source curve type: TBP at 760 mmHg • Mean API gravity DATA 35.0000 Volume percent distillated API gravity data .. Temperatures Volume percent.. \oplus 3.83000 98 °F • 12.0000 66.7000 5.00000 19.0000 125 °F 55.3000 0 10.0000 167 °F 40.0000 37.6000 æ 20.0000 227 °F 62.0000 27.0000 30.0000 291 °F 82.0000 19.0000 OPTIONS -40.0000 370 °F 50.0000 460 °F Mean API gravity • 60.0000 552 °F API gravity data curve • 70.0000 643 °F 80.0000 799 °F UNITS 90.0000 1023 °F Temperature °F -100.000 1440 °F Light ends... Convert > Options... Cancel

If light ends have been selected, click on "*Light ends*".

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Enter your experimental values for the volume percentage of light ends.



ſ	Assay characterization				- 0 X		
	Select the source curve type: TBP at 7	60 mmHg			•		
	DATA	Mean API gravity 35.0000					
	Paste data from clipboard	Volume percent distillated	Temperatures	Volume percent	API gravity data		
	 Insert a new line Delete the current line 	3.83000 5.00000	98 °F ▼ 125 °F	12.0000 19.0000	66.7000 55.3000		
e"	Draw graph	10.0000 20.0000 30.0000	167 °F 227 °F 201 °F	40.0000 62.0000 82.0000	37.6000 27.0000		
5.	OPTIONS	40.0000	370 °F 460 °F	02.0000	19.0000		
	API gravity data curve 🔻	60.0000 70.0000	552 °F 643 °F				
	UNITS	90.0000 100.000	1023 °F 1440 °F				
×	Options Light ends			Convert >	Cancel		

Click on "Options".

Select the number of pseudo-compounds					
you want to generate for the different	Options				x
temperature ranges.	Intervals Co	onversions			
Here, 29 pseudo compounds will be		Temperature i	ntervals for distillation o	tuts	
generated.	Values are	expressed in:	°F 🔻		
	Сору	Paste	🔇 Reset		
	T Min.	T Max.	Number of compou	Delta T	
	50	150	4	25	
	150	550	16		
	550	750	4		
	750	1250	5		
			Ok	Cance	
Click on " <i>OK</i> " to confi	rm. /				

Select the source curve type: TBP at	t 760 mmHg			•
		Mean API gravity		
	35.0000			
Copy data to clipboard				
Paste data from clipboard	Volume percent distillated	Temperatures	Volume percent	API gravity data
Insert a new line	3.83000	98 °F 🔻	12.0000	66.7000
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	10.0000	167 °F	40.0000	37.6000
🔀 Draw graph	20.0000	227 °F	62.0000	27.0000
	30.0000	291 °F	82.0000	19.0000
OPTIONS	40.0000	370 °F		
Mean API gravity 🔹	50.0000	460 °F	1	
A Di accusto dete essere	60.0000	552 °F	1	
API gravity data curve	70.0000	643 °F]	
	80.0000	799 °F		
	90.0000	1023 °F		
Temperature °F 🛛 💌	100.000	1440 °F		
Ontions Light ends			Convert	Cancel
Light ends			convert	cancer

Click on "Convert" to generate pseudo-compounds.

This window displays the data that was generated. 32 compounds will be taken into account:

- > 3 light ends already defined (C3, iC4 and nC4).
- > 29 pseudo compounds as explained before.

The user can plot graphs to analyze the results.

X axis:	Bubble points temperatures Molecular weights Specific gravity Molar fractions API degree Watson characterization factor VolumePercentOut
Y axes:	Molecular weights Specific gravity Holar fractions API degree Watson characterization factor VolumePercentOut
	Ok Cance

Assay characterization								3
				Number of p	oints			
	32.0000							
Copy data to clipboard								
Pasiz dala from tipboard	Bubble p	Molecula	Specific a	Molar fra	API degree	Watson c	VolumePe	
Insert a new line	-43,672 °F	0.0440956 k	0.506251	3.97384E-00	148.006	14.7457	9.00000E-00	
	10.904 °F	0.0581222 k	0.563782	5.59575E-00	119.483	13,7964	0.330000	
Delate the current tare	31.1 °F	0.0581222 k	0.584871	1.33516E-00	110,434	13,4865	0.825000	
🔀 Draw graph	37.037 °F	0.0590957 k	0.593720	3.59597E-00	106,828	13,3389	2.09448	1
	88.0953 °F	0.070319 kg	0.615489	1.46531E-00	98.3985	13.2937	3.45135	1
INITS	113.627 °F	0.0761553 k	0.630196	1.78813E-00	93.0333	13,1821	4.44188	1
	138.874 °F	0.0820988 k	0.655550	4.09439E-00	84.3493	12,8556	6.32442	1
Temperature	162.804 °F	0.087439 kg	0.691167	5.63134E-00	73.2263	12.3535	9.48892	1
Molar mass kg/mol 💌	187.48 °F	0.0927145 k	0.725036	6.38154E-00	63,6628	11,9300	13.4368	1
and the second se	212.462 °F	0.0984203 k	0.750741	6.10495E-00	56,9803	11.6679	17.6117	1
	237.447 °F	0.104667 kg	0.769632	5.69905E-00	52.3541	11,5209	21.6808	1
	262.449 °F	0.110815 kg	0.786762	5.38019E-00	48,3510	11,4032	25.6399	1
	287.323 °F	0.116887 kg	0.802102	4.91039E-00	44.9114	11.3121	29.4455	1
	312.263 °F	0.123266 kg	0.815079	4.27208E-00	42.1028	11,2545	32.9624	1
	337.319 °F	0.130053 kg	0.825714	3.76335E-00	39,8668	11,2285	36.1621	1
	362.429 °F	0.137257 kg	0.834442	3.37793E-00	38,0744	11,2265	39.1282	
	387.483 °F	0.144808 kg	0.841941	3.15887E-00	36,5641	11,2384	41.9667	1
	412.485 °F	0.152573 kg	0.849252	2.99971E-00	35,1172	11,2502	44.7619	
	437.469 °F	0.160558 kg	0.856456	2.84402E-00	33,7157	11,2611	47.5310	
	462.491 °F	0.168803 kg	0.863526	2.69790E-00	32.3631	11.2718	50.2702	
	487.499 °F	0.177297 kg	0.870476	2.58285E-00	31,0548	11,2820	52.9912	
	512.5 °F	0.186053 kg	0.877324	2.47910E-00	29.7859	11,2916	55.7079	
	537.501 °F	0.19509 kg/	0.884064	2.38318E-00	28.5562	11.3007	58.4242	
	575.044 °F	0.209218 kg	0.894010	4.54398E-00	26.7756	11,3135	62.5292	
	624.889 °F	0.22908 kg/	0.906974	4.15989E-00	24.5132	11,3281	67.9896	
	672.804 °F	0.250106 kg	0.917671	2.58425E-00	22,6946	11,3585	72.5226	-
	724.734 °F	0.276402 kg	0.925398	1.88082F-00	21.4072	11.4333	75.7928	4
						OF	Cancel	



Example of graph: Example of graph: molecular weights (MW) vs. bubble points temperatures.



At this stage, it is important to save the composition of the mixture. This composition will be required afterward to carry out simulations or compute mixture properties. Once this window is closed, it will no longer be possible to access the composition.

- -Assay characterization Number of points DATA 32.0000 Copy data to clipboard Nolecula... Specific g... Molar fra... API degree Watson c... Bubble p... VolumePe. -43.672 °F 0440956 k 0.506251 3.97384E-00 148.006 14,7457 9.00000E-00 10.904 °F 0581222 k 0.563782 5.59575E-00 119.483 13,7964 0.330000 9 31.1 °F 0.825000 581222 k 0.584871 1.33516E-00 110.434 13,4865 2×C Draw graph... 37.037 °F 0.0590957 k 0.593720 3.59597E-00 106.828 13.3389 2.09448 88.0953 °F 0.070319 kg 0.615489 1.46531E-00 98,3985 13.2937 3,45135 113.627 °F 0.0761553 k 0.630196 1.78813E-00 93,0333 13,1821 4,44188 LINITS 138.874 °F 0.0820988 k 0.655550 4.09439E-00 84.3493 12,8556 6.32442 Temperature 162.804 °F 0.087439 kg 0.691167 5.63134E-00 73.2263 12.3535 9,48892 kg/mol -Molar mass 187.48 °F 0.0927145 k 0.725036 6.38154E-00 63.6628 11.9300 13,4368 212.462 °F 0.0984203 k 0.750741 6.10495E-00 56.9803 11,6679 17.6117 237,447 °F 0.104667 kg 0.769632 5.69905E-00 52.3541 11.5209 21.6808 5.38019E-00 48.3510 11,4032 25,6399 262.449 °F 0.110815 kg 0.786762 287.323 °F 0.116887 kg 0.802102 4.91039E-00 44.9114 11,3121 29,4455 312.263 °F 0.123266 kg 0.815079 4.27208E-00 42.1028 11,2545 32.9624 337.319 °F 0.130053 kg 0.825714 3.76335E-00 39.8668 11.2285 36.1621 362.429 °F 0.137257 kg 0.834442 3.37793E-00 38.0744 11,2265 39.1282 3.15887E-00 36.5641 11,2384 41.9667 387.483 °F 0.144808 kg 0.841941 412.485 °F 0.152573 kg 0.849252 2.99971E-00 35.1172 11,2502 44.7619 11,2611 437.469 °F 0.160558 kg 0.856456 2.84402E-00 33.7157 47.5310 462.491 °F 0.168803 kg 0.863526 2.69790E-00 32.3631 11,2718 50.2702 487,499 °F 0.177297 kg 0.870476 2.58285E-00 31.0548 11,2820 52.9912 512.5 °F 0.186053 kg 0.877324 2,47910E-00 29,7859 11.2916 55,7079 2.38318E-00 28.5562 11.3007 58,4242 537.501 °F 0.19509 kg/ 0.884064 575.044 °F 0.209218 kg 0.894010 4.54398E-00 26.7756 11.3135 62.5292 624.889 °F 0.22908 kg/ 0.906974 4.15989E-00 24.5132 11.3281 67.9896 672.804 °F 0.250106 kg 0.917671 2.58425E-00 22,6946 11,3585 72.5226 724 734 °F 0 276402 kg 0 925398 1.88082F-00 21.4072 11.4333 75,7928 Ok Cancel

Click on the table

Click on « Copy data to clipboard » in order to paste the table into Excel or paste the composition into a feed module of ProSimPlus

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Pseud

FILE

Click on "*OK*" to close this window and come back to the Petroleum Cut window.

📋 Copy data t		Number of points						
	clipboard	22,0000				_	_	_
1 000 mm		_	-					
-		Bubble p	Molecula	Specific g	Molar fra	API degree	Watson c	VolumePe.,
		-43.672 °F	0.0440956 k	0.506251	3.97384E-00	148,006	14.7457	9.00000E-00
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Diaw graph		37.037 °F	0.0590957 k	0.593720	3.59597E-00	106,828	13,3389	2.09448
		88.0953 °F	0.070319 kg	0.615489	1.46531E-00	98.3985	13,2937	3.45135
UNITS		113.627 *F	0.0761553 k	0.630196	1.78813E-00	93.0333	13.1821	4.44188
-		138.874 °F	0.0820988 k	0.655550	4.09439E-00	84.3493	12.8556	6.32442
remperature		162.804 °F	0.087439 kg	0.691167	5.63134E-00	73,2263	12.3535	9.48892
Molar mass k	a/mol 👻	187.48 *F	0.0927145 k	0.725036	6.38154E-00	63.6628	11,9300	13.4368
		212.462 *F	0.0984203 k	0.750741	6.10495E-00	56.9803	11.6679	17.6117
		237.447 °F	0.104667 kg	0.769632	5.69905E-00	52.3541	11,5209	21.6808
		262.449 °F	0.110815 kg	0.786762	5.38019E-00	48.3510	11,4032	25.6399
		287.323 *F	0.116887 kg	0.802102	4.91039E-00	44.9114	11.3121	29,4455
		312.263 °F	0.123266 kg	0.815079	4.27208E-00	42.1028	11.2545	32.9624
		337.319 °F	0.130053 kg	0.825714	3.76335E-00	39,8668	11,2285	36.1621
		362.429 °F	0.137257 kg	0.834442	3.37793E-00	38.0744	11,2265	39.1282
		387.483 *F	0.144808 kg	0.841941	3.15887E-00	36.5641	11,2384	41.9667
		412.485 °F	0.152573 kg	0.849252	2.99971E-00	35.1172	11.2502	44.7619
		437.469 °F	0.160558 kg	0.856456	2.84402E-00	33,7157	11,2611	47.5310
		462.491 °F	0.168803 kg	0.863526	2.69790E-00	32,3631	11,2718	50.2702
		487.499 *F	0.177297 kg	0.870476	2.58285E-00	31.0548	11.2820	52.9912
		512.5 °F	0.186053 kg	0.877324	2.47910E-00	29,7859	11,2916	55.7079
		107.501.1F	0.19509 kg/	0.884064	2.38318E-00	28.5562	11.3007	58,4242
		575.044 'F	0.20700	0.894010	4.54398E-00	26.7756	11.3135	62.5292
		624.889 °F	0.22908 kg/	0.906974	FOROF	24.5132	11.3281	67.9896
		672,804 °F	0.250106 kg	0.917671	2.584251	42.6946	11.3585	72.5226
		724.734 °F	0.276402 km	0.975398	1.88082F-00	21.4072	11.4333	75.7928
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PETROLEUM CUT	Use this window to create pseu	udo-compounds for a petroleum cut.	
pad	Select 2 or 3 known parameters		
ave as	 Normal boiling point Molecular weight 		
aste data from clipboard	Watson characterization fa API Degree	ctor	
elete the current lin .	Specific gravity		
^	Data		_
rature °C 👻	Normal boiling point	Molecular weight	-
	275.948 K	59.0957 g/mol	
ilar weight g/mol 👻	304.314 K	70.319 g/mol	
	318.498 K	76.1553 g/mol	
	332.524 K	82.0988 g/mol	
	345.819 K	87.439 g/mol	
	359.528 K	92.7145 g/mol	
	373.407 K	98.4203 g/mol	
	387.287 K	104.667 g/mol	
	401.177 K	110.815 g/mol	_
	414.996 K	116.887 g/mol	
	428.852 K	123.266 g/mol	_
	442.772 K	130.053 g/mol	_
	456.722 K	137.257 g/mol	
	470.641 K	144.808 g/mol	-
	484.531 K	152.573 g/mol	_

Select 2 or 3 parameters that will be used for the calculation of physical properties. In this example, select:

- > normal boiling point.
- molecular weight.

Click on "*Generate*" to create the pseudo-compounds.

The pseudo-compounds have been automatically generated.

They are named "NBP-" (for Normal Boiling Point) followed by the value expressed in Kelvin.

COMPOUNDS This window helps you to manage a compound list. FILE Image: manage a compound list. Image: manage a compound list. Image: manage a compound list. Image: manage a compound list. Image: manage a compound list. Image: manage a compound list. Image: manage a compound list. Image: manage a compound list. Image: manage a compound list. Image: manage a compound list. Image: manage a compound list. Image: manage a compound list. Image: manage a compound list. Image: manage a compound list. Image: manage a compound list. Image: manage a compound list. Image: manage a compound list. Image: manage a compound list. Image: manage a compound list. Image: manage a compound list. Image: manage a compound list. Image: manage a compound list. Image: manage a compound list. Image: manage a compound list. Image: manage a compound list. Image: manage a compound list. Image: manage a compound list. Image: manage a compound list. Image: manage a compound list. Image: manage a compound list. Image: manage a compound list. Image: manage a compound list. Image: manage a compound list. Ima	
FILE # TUPAC Name Registry Cas Number	
[↑] Open ¹ PROPANE ⁷⁴⁻⁹⁸⁻⁶ [™] Save as ¹ ISOBUTANE ⁷⁵⁻²⁸⁻⁵ [™] Publish ¹ NBP-376(K) ¹ 106-97-8 [™] PACKAGE [•] NBP-304(K) ¹ NBP-333(K) ¹ 106-97-8 [™] EDIT [•] NBP-318(K) ¹ NBP-333(K) [®] Select compounds ¹ NBP-350(K) ¹ NBP-373(K) ¹ NBP-337(K) [®] Add a new compound ¹ NBP-318(K) ¹ NBP-401(K) [®] Remove all the compounds ¹ NBP-415(K) ¹ NBP-429(K) [®] Clone this compound ¹ NBP-429(K) ¹ NBP-443(K)	
Image: Save as 2 ISOBUTANE 75-28-5 Image: Publish 3 n-BUTANE 106-97-8 Image: Publish 4 NBP-276(K) 5 Image: Publish 5 NBP-304(K) 6 Image: Publish 6 NBP-318(K) 7 Image: Publish 7 NBP-333(K) 8 Image: Publish 7 NBP-333(K) 8 Image: Publish 7 NBP-333(K) 8 Image: Publish 9 NBP-360(K) 8 Image: Publish 9 NBP-360(K) 10 Image: Publish 9 NBP-373(K) 11 Image: Publish 10 NBP-373(K) 11 Image: Publish 10 NBP-401(K) 13 Image: Publish 13 NBP-415(K) 14 Image: Publish 15 NBP-443(K) 15	П
3 n-BUTANE 106-97-8 Publish 4 NBP-276(K) S NBP-304(K) PACKAGE 6 NBP-318(K) 7 NBP-333(K) 8 NBP-346(K) 9 NBP-360(K) 10 NBP-373(K) 11 NBP-387(K) 11 NBP-401(K) 13 NBP-415(K) 14 NBP-429(K) 15	
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EDIT 7 NBP-333(K) Select compounds 9 NBP-346(K) Select compounds 9 NBP-360(K) Edit this compound 10 NBP-373(K) Add a new compound 12 NBP-401(K) Remove all the compounds 13 NBP-429(K) Clone this compound 15 NBP-443(K)	
8 NBP-346(K) 9 NBP-360(K) 9 NBP-373(K) 10 NBP-373(K) 11 NBP-387(K) 12 NBP-401(K) 13 NBP-415(K) 14 NBP-429(K) 15 NBP-443(K)	
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17 NBP-471(K)	
SERVICES 18 NBP-485(K)	
19 NBP-498(K)	
Create a pseudo-compound 20 NBP-512(K)	
Temperature dependent properties 21 NBP-526(K)	
Editor array 22 NBP-540(K)	
23 NBP-554(K)	
Compare with the original 24 NBP-575(K)	
Compare the compounds 25 NBP-603(K)	
26 NBP-629(K)	
MODIFICATIONS Comments :	
Move this compound up	
Wove this compound down Ok Cance	I

You can access physical properties by double clicking on a pseudocompound.





The Compound Editor window allows you to browse through the properties generated for each compound. Some properties can be plotted on a graph (in this example, the vapor pressure of the pseudo-compound NBP-360(K)).

It is also possible to compare temperature dependant properties between different compounds

Edit compounds		
COMPOUNDS	This window helps you to man	nage a compound list.
FILE 🔺	# IUPAC Name	Registry Cas Number
🔄 Open	1 PROPANE	74-98-6
Enve ar	2 ISOBUTANE	75-28-5
Jave as	3 n-BUTANE	106-97-8
Publish	4 NBP-276(K)	
	5 NBP-304(K)	
PACKAGE — 🗸	6 NBP-318(K)	
	7 NBP-333(K)	
	8 NBP-346(K)	
Select compounds	9 NBP-360(K)	
Fdit this compound	10 NBP-373(K)	
	11 NBP-387(K)	
Add a new compound	12 NBP-401(K)	
Remove all the compounds	13 NBP-415(K)	
	14 NBP-429(K)	
Clone this compound	15 NBP-443(K)	
X Delete the selection	16 NBP-457(K)	
	17 NBP-471(K)	
SERVICES A	18 NBP-485(K)	
Create a pseudo-compound	19 NBP-498(K)	
	20 NBP-512(K)	
🛛 Temperature dependent properties	21 NBP-526(K)	
Editor array	22 NBP-540(K)	
,	23 NBP-554(K)	
Compare with the original	24 NBP-575(K)	
Compare the compounds	25 NBP-603(K)	
	26 NBP-629(K)	
	Comments :	
ORDER		
Move this compound up		
A Mousthic compound down		Ok Canad
Wove this compound down		OK Cancel

1. Select "*atm*" for pressure and "°*F*" for temperature.

2. Select "Vapor pressure".

3. Select the compounds that will be used for the comparison. Here we check "*All*" to select all compounds, then uncheck the four heaviest ones.

4. Enter the temperature range: 100°C to 200°C.

- O X Temperature dependent properties TEMPERATURE DEPENDANT This window helps you to compare the same temperature dependent property of several compounds. PROPERTIES Data Chart Grid ACTIONS 2×C Calculate and plot Property D Unit system apor pressure Compounds T Name 1 NBP-575(K) CHART NBP-603(K) Lines 1 NBP-629(K) Points J NBP-658(K) Legend NBP-699(K) NBP-754(K) NBP-810(K) = NBP-865(K) NBP-969(K) All / None Temperature bounds Number of points Specify the temperature bounds [TMin, TMax] 20 Temperature min. Temperature max. 100 °C 200 °C Use the temperature bounds of the compounds Close

5. When all parameters are defined, click on *"Calculate and plot"*.

Click on the "Chart" tab to view the graph.



Check the "Logarithmic scale" option.

Step 5: Paste the mixture composition into the application that is used

The table that includes the mixture composition has been copied in the step 3. You can now paste it into the application you are using.

If you are using Simulis Thermodynamics in Excel:

Copy the table into the Excel spreadsheet. The "Molar fractions" column corresponds to the mixture composition.

FILE	HOME INSERT PAGE LAYO	JT FORMULAS	DATA REVIEV	V VIEW DEV	ELOPER A	DD-INS Custom Macro	
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Clipb	oard 19 Font		Aligne	nent	ra Ni	imber is	
M29	\cdot : $\times \checkmark f_x$						
A	В	с	D	E	F	G	
1							
2							
3	Bubble points temperatures	Molecular weights	Specific gravity	Molar fractions	PI degree	Watson characterization factor	
4	-43.672 °F	0.0440956 kg/mol	0.50625104	0.003973842	148.0055935	14.7456688	
5	10.904 °F	0.0581222 kg/mol	0.563782333	0.00559575	119.4833889	13.796359	
6	31.1 °F	0.0581222 kg/mol	0.584870743	0.013351639	110.4337975	13.4865056	
7	37.037 °F	0.0590957 kg/mol	0.593719678	0.035959719	106,8279607	13.3388579	
8	88.0953 *F	0.070319 kg/mol	0.61548901	0.014653073	98.39849966	13.2936590	
9	113.627 °F	0.0761553 kg/mol	0.630196024	0.017881326	93.03331137	13.1820851	
10	138.874 *F	0.0820988 kg/mol	0.65555007	0.040943872	84.34926212	12.855611	
11	162.804 *F	0.087439 kg/mol	0.69116679	0.056313386	73.22627078	12.353524	
12	187.48 °F	0.0927145 kg/mol	0.725035666	0.063815434	63.66281276	11.9300474	
13	212.462 *F	0.0984203 kg/mol	0.75074144	0.061049453	56.98033703	11.6679471	
14	237.447 °F	0.104667 kg/mol	0.76963195	0.056990482	52.35411302	11.5208777	
15	262.449 °F	0,110815 kg/mol	0.786762393	0.053801903	48.35099505	11.4031828	
16	287.323 *F	0.116887 kg/mol	0.802102342	0.049103901	44.91140371	11.3120756	
17	312.263 °F	0.123266 kg/mol	0.815079233	0.042720759	42.10275457	11.2545134	
18	337.319 °F	0.130053 kg/mol	0.82571401	0.037633485	39.86683859	11.2284827	
19	362.429 *F	0.137257 kg/mol	0.834442193	0.033779329	38.07435905	11.2265177	
20	387,483 *F	0.144808 kg/mol	0.841940763	0.031588744	36.56408039	11.2384334	
21	412,485 *F	0.152573 kg/mol	0.84925219	0.029997053	35.11717236	11.2502249	
22	437.469 *F	0.160558 kg/mol	0.85645598	0.028440201	33.7157298	11.2611174	

If you are using Simulis Thermodynamics within ProSimPlus:

In the configuration window of the feed module, select "Mole fractions" for the flowrate specification, then right click in the table to paste the mixture composition.









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