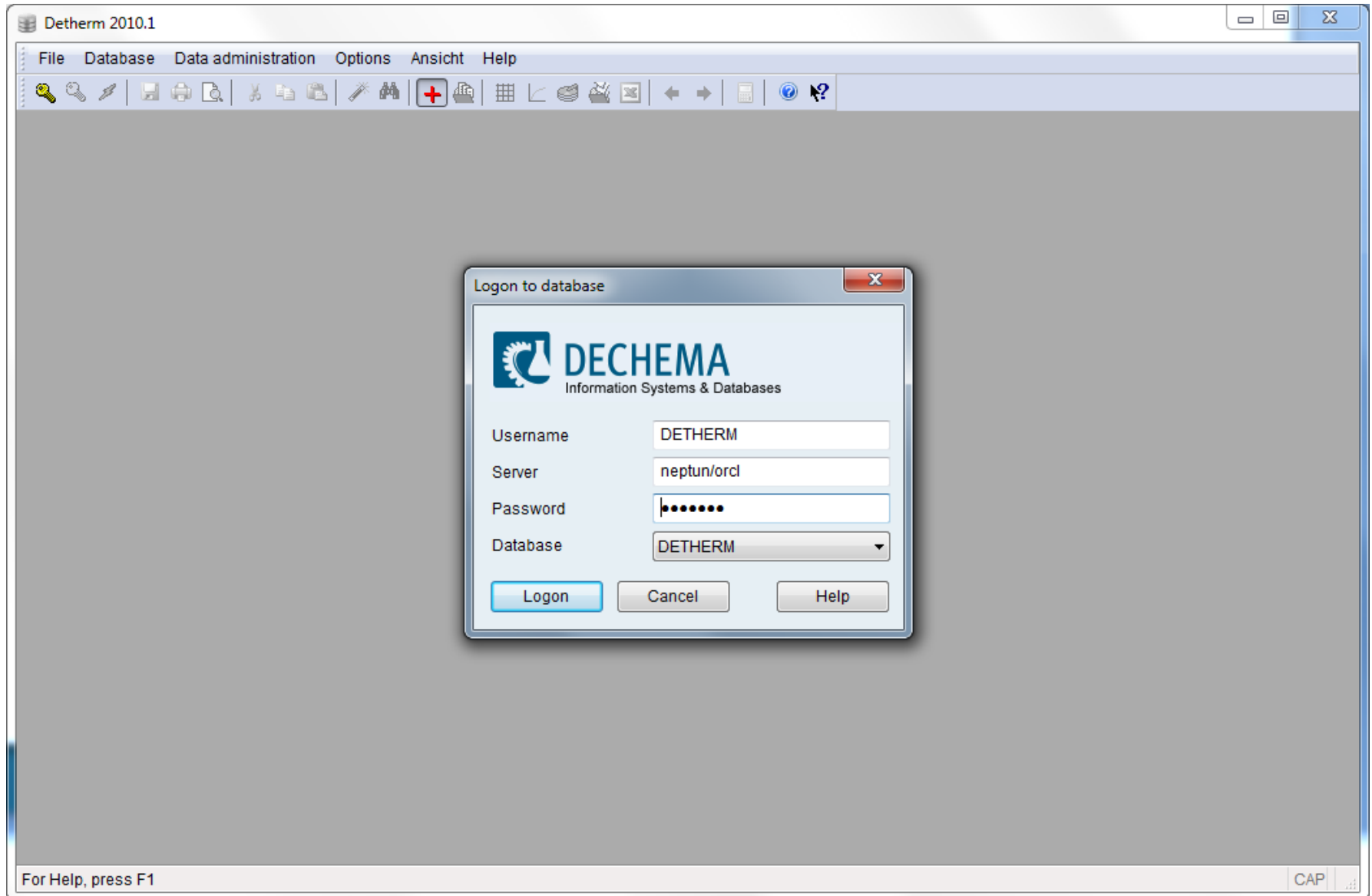




DEThERM in Action ...

Overview on the usage of DETHERM

1st step: Logon to database server



Wizard-Search: Identification of component(s)

The screenshot shows the Detherm 2010.1 Wizard-Search window. The search term 'dimethylsul' is entered in the search box. The results table lists various chemical compounds with their systematic names, sum formulas, and CAS numbers. A yellow starburst graphic is overlaid on the left side of the window, and a blue pencil icon is also present.

1. Please enter the searched mixture respectively substance

dimethylsul

Hit	Systematic name	Sum Formula	CAS No
dimethylsulfoxide	sulfinylbismethane	C2H6OS	67-68-5
dimethylsulfur diimide	dimethylsulfur diimide	C2H6N2S	13849-02-0
dimethyltetraphenylcyclotrisiloxane	2,2-dimethyl-4,4,6,6-tetraphenylcyc...	C26H26O3Si3	1438-86-4
dimethylthallium iodide	iododimethylthallium	C2H6ITI	7066-67-3
dimethylthioborinic acid methyl ester	dimethylthioborinic acid methyl ester	C3H9BS	19163-05-4
dimethylthiodipropionate	3,3'-thiobispropanoic acid dimethyl...	C8H14O4S	4131-74-2
dimethylthioformamide	N,N-dimethylmethanethioamide	C3H7NS	758-16-7
dimethyltin difluoride	difluorodimethylstannane	C2H6F2Sn	3582-17-0
dimethylurea	dimethylurea	C3H8N2O	1320-50-9
dimethylurea compd. with sulfuric a...	dimethylurea compd. with sulfuric ...	C3H10N2O5S	D907230930
dimethylurea compd. with sulfuric a...	dimethylurea compd. with sulfuric ...	C9H26N6O7S	D907220929
dimethylvinylborane	ethenyldimethylborane	C4H9B	5846-37-7

Mixture(s) with to components, consisting of ...

For Help, press F1

Result: Properties of Dimethylsulfoxide in overview

Detherm 2010.1

File Database Data Edit Options Ansicht Window Help

Systems & properties

Pure components

- DMSO
 - 2nd virial coefficient (G)
 - acentric factor
 - autoignition temperature
 - boiling temperature
 - boiling temperature (L)
 - complex permittivity, imaginary part (L)
 - complex permittivity, real part (L)
 - critical compressibility factor
 - critical density
 - critical pressure
 - critical temperature
 - critical volume
 - cubic expansion coefficient (L)
 - density (L)
 - density (S)
 - dielectric constant
 - dielectric constant (L)
 - diffusion coefficient (L)
 - dipole moment
 - enthalpy
 - enthalpy of combustion
 - enthalpy of formation
 - enthalpy of formation (G)
 - enthalpy of formation (L)
 - enthalpy of fusion
 - enthalpy of sublimation
 - enthalpy of vaporization

DMSO: Properties in overview

Property	N...	N...	>= K	<= K	>= Pa	<= Pa
2nd virial coefficient (G)	4	17	293.15	3623.00		
acentric factor	4	4	720.00	720.00	5700000.00	5704597.50
autoignition temperature	1	1				
boiling temperature	2	2	461.92	462.19	101325.00	101325.00
boiling temperature (L)	7	10	313.15	463.35	101300.00	101300.00
complex permittivity, imaginary part (L)	2	0				
complex permittivity, real part (L)	2	0				
critical compressibility factor	4	4	707.00	720.00	5700000.00	5847000.00
critical density	1	1	720.00	720.00	5700000.00	5700000.00
critical pressure	8	8	707.00	720.00	5650000.00	5950000.00
critical temperature	8	8	707.00	738.00	5700000.00	5847000.00
critical volume	4	4	707.00	738.00	5847000.00	5847000.00
cubic expansion coefficient (L)	2	6	293.15	313.15		
density (L)	266	816	288.15	729.00	100000.00	101325.00
density (S)	2	2	278.15	278.15		
dielectric constant	1	1				
dielectric constant (L)	64	181	288.15	523.15	100000.00	50000000.00
diffusion coefficient (L)	2	7	288.15	328.15		
dipole moment	6	6				
enthalpy	1	0				
enthalpy of combustion	1	1				
enthalpy of formation	1	1				

Display Plot

For Help, press F1

CAP

Liquid Density of Dimethylsulfoxide: f(t,p)

Detherm 2010.1

File Database Data Edit Options View Window Help

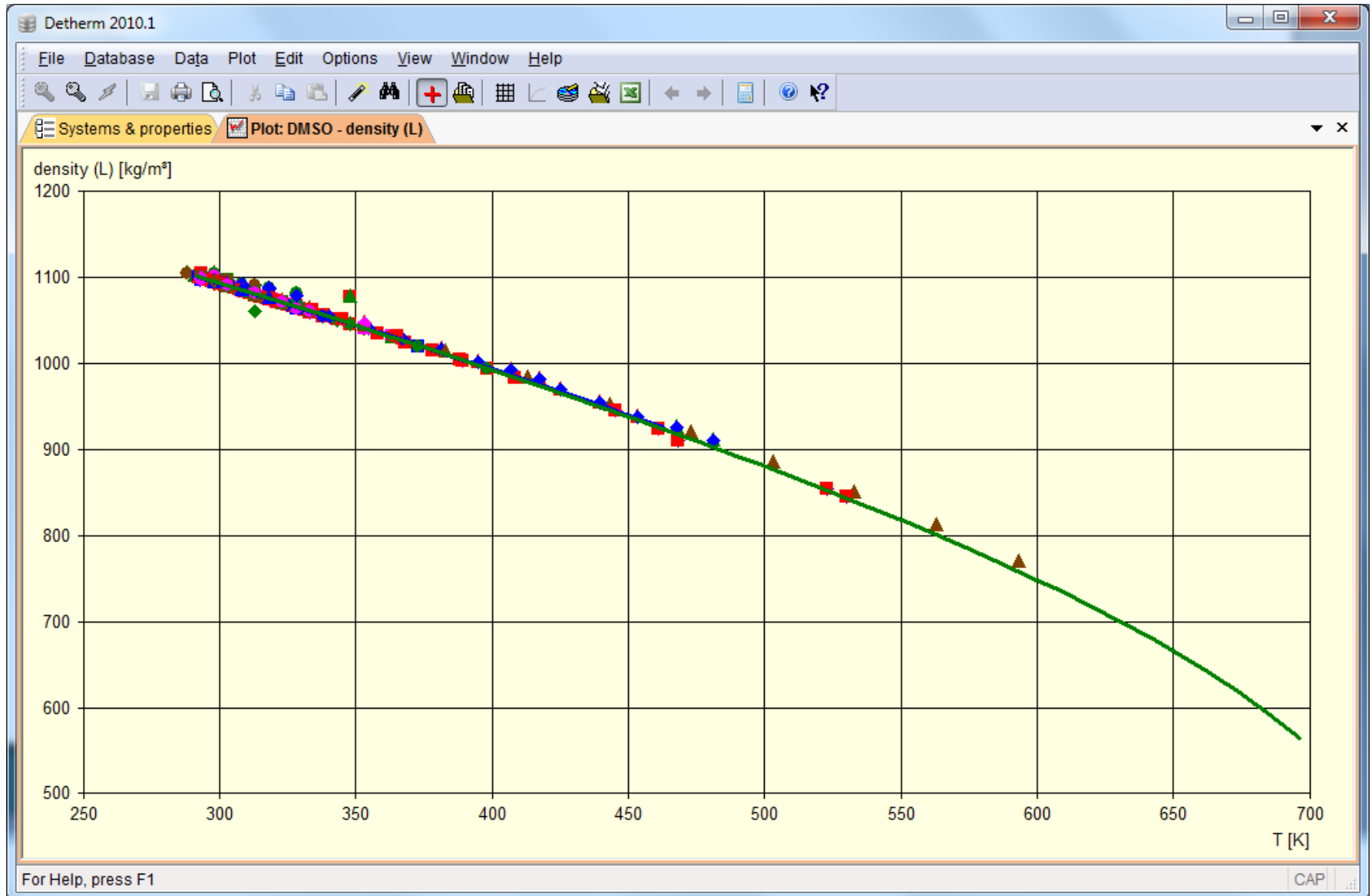
Systems & properties Table: DMSO - density (L)

Line no.	T		p		density		Table No	UTI	Source no.
	System		System		System				
	K	± K	Pa	kg/m ³	± kg/m ³	L			
121	297.15				1096.370				
122	299.15				1094.378				
123	301.15				1092.430				
124	303.15				1090.423				
125	305.15				1088.420				
126	307.15				1086.397				
127	309.15	± 0.0050000		-	1084.407	± 2.0000E-002	11	46	DDB-PCP:2007-DEC/125027
128	311.15				1082.404				
129	313.15				1080.430				
130	315.15				1078.421				
131	317.15				1076.425				
132	319.15				1074.400				
133	321.15				1072.427				
134	323.15				1070.447				

(44) ID: PRP-4696i.1982
 Author(s): Bicknell,R.T.M.; Davies,D.B.; Lawrence,K.G.
 Titel: Density, Refractive Index, Viscosity and H Nuclear Magnetic Resonance Measurements of Dimethyl Sulfoxide at 2 C Intervals in the Range 20-60 C
 Journal: J. Chem. Soc. Faraday Trans. I
 CODEN: JCFTAR
 Volume: 78
 published: 1982
 Pages: 1595-1601
 DOI: <http://dx.doi.org/10.1039/f19827801595>
 Segment: DDB

For Help, press F1

Density of Dimethylsulfoxide: Plot of temperature dependency



Density of Dimethylsulfoxide: Excel-Export of data (1)

The screenshot shows the Detherm 2010.1 interface with a table of density data for DMSO. The table has columns for Line no., Temperature (K), Pressure (Pa), Density (kg/m³), and Source no. An 'Excel-Export' button is highlighted with a red circle, and a tooltip indicates 'Export of the selected data to MS-Excel'.

Line no.	T (K)	p (Pa)	density (kg/m³)	UTI	Source no.
1	298.15		1095.800	1	1
2	293.15		1100.830		
3	298.15		1095.660		
4	303.15		1090.650		
5	308.15		1085.690		
6	313.15		1080.580	* 3	2
7	318.15		1075.590		
8	323.15		1070.500		
9	328.15		1065.560		
10	298.15		1095.400	1 * 4	3
11	298.15		1095.332	* 5	3
12	293.15		1100.000		
13	313.15		1082.500	6	4
14	333.15		1063.700		

+++ Table definition +++
 Column No. 1 temperature
 Column No. 2 pressure
 Column No. 3 density (L)

+++ Substance and/or mixture identification +++
 DMSO

Export of the selected data to MS-Excel

Density of Dimethylsulfoxide: Excel-Export of data (2)

	A	B	C	D	E
1	System:	DMSO			
2	Component:	DMSO			
3	CAS-No.:	67-68-5			
4	Sum formula:	C2H6OS			
5	Mol weight [g/mol]:	78,1338			
6					
7	temperature	pressure	density (L)	Collection:	UTI:
8	[K]	[Pa]	[kg/m ³]		
9					
10	298,15		1095,8	DDB	DDB-PURE:2005-JUL/2000151
11					
12	293,15		1100,83	DDB	DDB-PCP:2007-DEC/8859
13	298,15		1095,66	DDB	DDB-PCP:2007-DEC/8859
14	303,15		1090,65	DDB	DDB-PCP:2007-DEC/8859
15	308,15		1085,69	DDB	DDB-PCP:2007-DEC/8859
16	313,15		1080,58	DDB	DDB-PCP:2007-DEC/8859
17	318,15		1075,59	DDB	DDB-PCP:2007-DEC/8859
18	323,15		1070,5	DDB	DDB-PCP:2007-DEC/8859
19	328,15		1065,56	DDB	DDB-PCP:2007-DEC/8859
20					
21	298,15		1095,4	DDB	DDB-PCP:2007-DEC/12076
22					
23	298,15		1095,332	DDB	DDB-PCP:2007-DEC/12077
24					
25	293,15		1100	DDB	DDB-PCP:2007-DEC/126823
26	313,15		1082,5	DDB	DDB-PCP:2007-DEC/126823
27	333,15		1063,7	DDB	DDB-PCP:2007-DEC/126823
28	353,15		1047,2	DDB	DDB-PCP:2007-DEC/126823


Search for pure, binary and ternary data of DMSO, THF, water

Detherm 2010.1

File Database Data administration Options Ansicht Help

DETERM Wizard-Search

1. Please enter the searched mixture respectively substance



Hit	Systematic name	Sum Formula	CAS No
water	water	H2O	7732-18-5
water dimer	water dimer	H4O2	25655-83-8
water dimer ((H2O)2)	water dimer	H4O2	25655-83-8
water-(3)H	water-t2	OT2	14940-65-9
water-d	water-d	DHO	14940-63-7
water-d-O17	water-d-O17	DHO	25372-56-9
water-d-O18	water-d-O18	DHO	20273-01-2
water-d-t	water-d-t	DOT	20272-95-1
water-d1	water-d	DHO	14940-63-7
water-d2	water-d2	D2O	7789-20-0
water-d2-O17	water-d2-O17	D2O	20205-58-7
water-d2-O18	water-d2-O18	D2O	14674-67-0

Mixture(s) with 1 to 3 components, consisting of ...

DMSO
THF
water

< Back Forward > Search Cancel Help

For Help, press F1

CAP

Result: Ternary LLE Data

The screenshot shows the Detherm 2010.1 software interface. The left pane displays a tree view under 'Systems & properties' with the following structure:

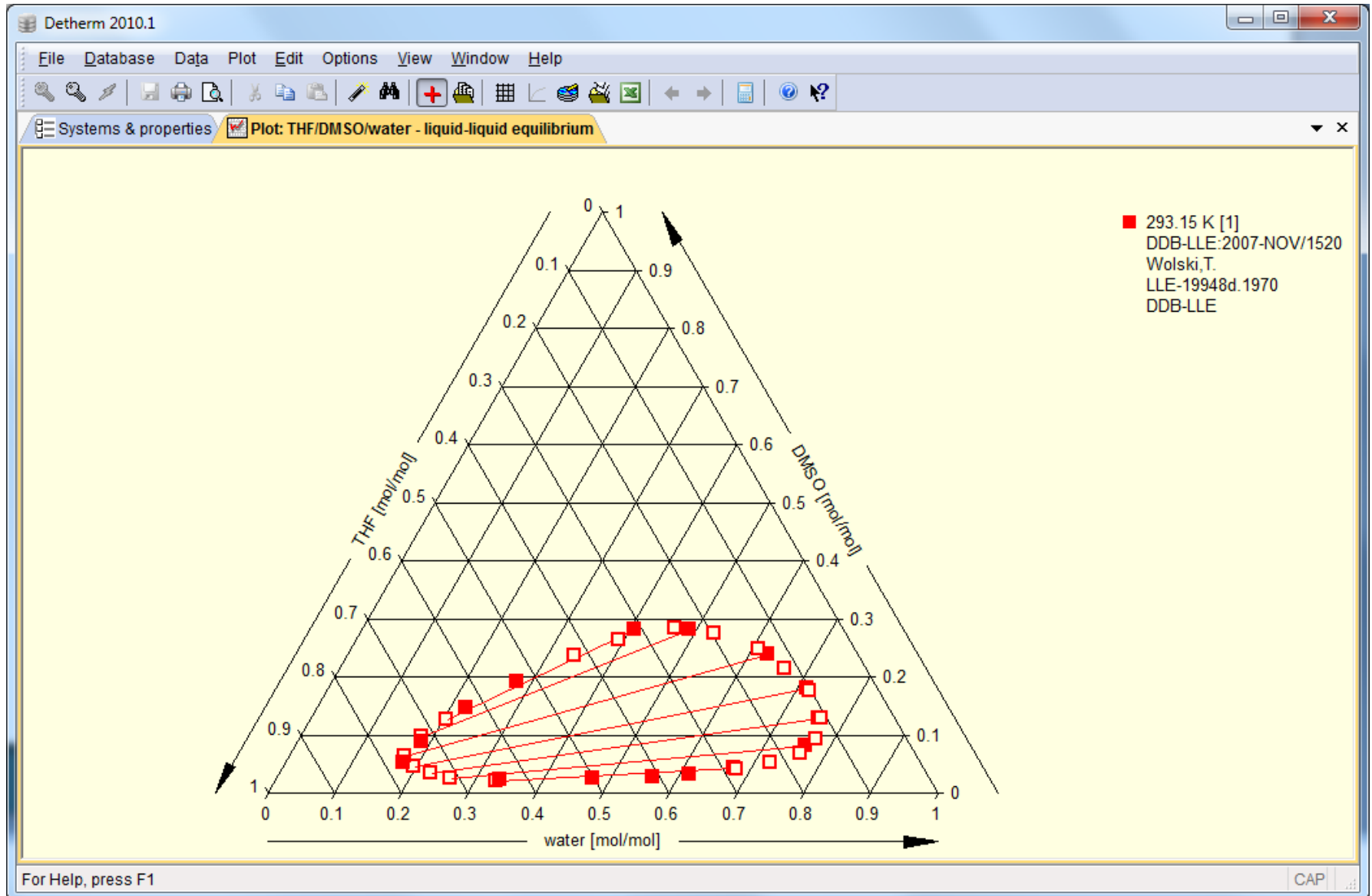
- Pure components
 - DMSO
 - THF
 - water
- 2-comp.-mixtures
 - DMSO/water
 - THF/DMSO
 - THF/water
- 3-comp.-mixtures
 - THF/DMSO/water
 - liquid-liquid equilibrium

The right pane displays the selected system: 'THF/DMSO/water: liquid-liquid equilibrium'. Below this, a table shows the following data:

No.	Property	C...	Year	Author(s)	temp...	p..	Data co...
1	Liquid-liquid equilibrium data	27	1970	Wolski,T.	293.15		DDB-LLE

Buttons for 'Display' and 'Plot' are located at the bottom of the right pane. The status bar at the bottom left reads 'For Help, press F1' and the bottom right shows 'CAP'.

Result: Plot of this ternary LLE data



Example for binary VLE-Data of DMSO/Water

Detherm 2010.1

File Database Data Edit Options Ansicht Window Help

Systems & properties Plot DMSO/water - vapor-liquid equilibrium, isothermal

activity coefficient (infinite dilution) (L)
 activity coefficient (L)
 cubic expansion coefficient (L)
 density (L)
 dielectric constant
 dielectric constant (L)
 enthalpy of dilution (L)
 enthalpy of mixing (L)
 enthalpy of solution (L)
 eutectic
 fusion temperature
 heat capacity (cp) (L)
 heat capacity (cp, excess) (L)
 isentropic compressibility (L)
 isothermal compressibility (L)
 no azeotrope under specified conditions
 refractive index, Na-D-line (L)
 solid-liquid equilibrium
 sound velocity (L)
 specific volume (L)
 specific volume, infinite dilution (L)
 surface tension
 surface tension (L)
 thermal conductivity (L)
 total complex permittivity, imaginary part
 total complex permittivity, real part
 vapor-liquid equilibrium
 vapor-liquid equilibrium, isobaric
 vapor-liquid equilibrium, isothermal

DMSO/water: vapor-liquid equilibrium, isothermal

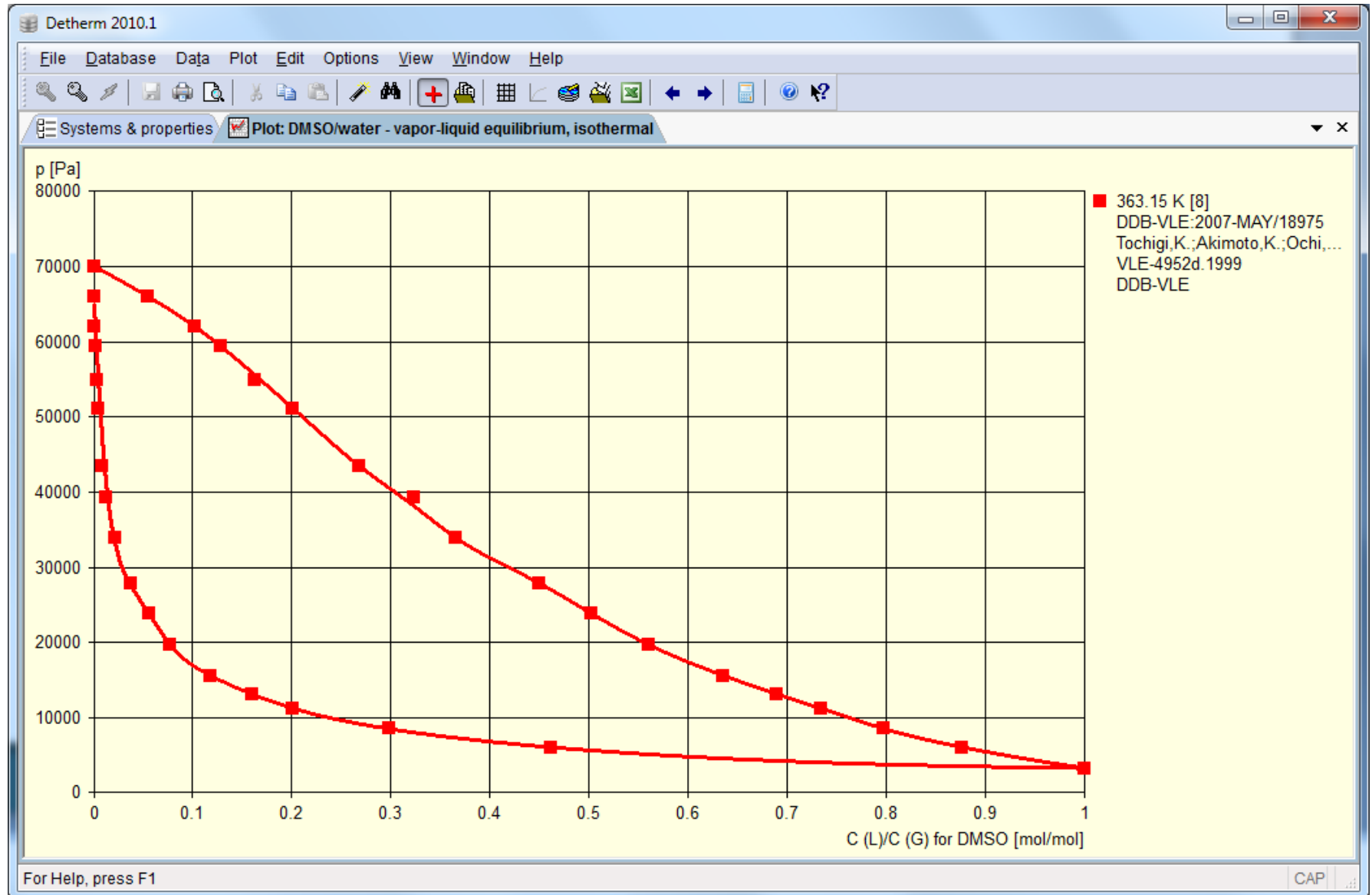
No.	Property	C...	Year	Author(s)	temperature [K]	pressure [Pa]	Data co...
1	Isothermal VLE-data (...)	11	1960	Kenttaemaa,J.;Lindbe...	343.15	1246.56 ... 31157.44	DDB-VLE
2	Isothermal VLE-data (...)	22	1976	Chan,T.C.;van Hook,W...	298.15 ... 343.15	78.66 ... 31170.78	DDB-VLE
3	Isothermal VLE-data (...)	9	1979	Taraszewska,J.;Klon...	298.15	81.33 ... 3166.41	DDB-VLE
4	Isothermal VLE-data (...)	11	1975	Biswas,S.;Gupta,A.R.	298.15	82.66 ... 3166.41	DDB-VLE
5	Isothermal VLE-data (...)	18	1974	Lam,S.Y.;Benoit,R.L.	298.15	79.99 ... 3170.41	DDB-VLE
6	Isothermal VLE-data (...)	79	1995	Lai,J.T.W.;Lau,F.W.;Ro...	296.09 ... 298.15	67.99 ... 3167.74	DDB-VLE
7	Isothermal VLE-data (...)	51	1995	Qian,X.;Han,B.;Liu,Y.;Y...	288.15 ... 303.15	50.66 ... 4243.65	DDB-VLE
8	Isothermal VLE-data (...)	18	1999	Tochigi,K.;Akimoto,K.;...	363.15	3279.73 ... 70070.25	DDB-VLE
9	vapor-liquid equilibriu...	18	1974	Lam,S.Y.;Benoit,R.L.	298.15	79.86 ... 3170.41	ELDAR
10	vapor-liquid equilibriu...	45	1995	Lai,J.T.W.;Lau,F.W.;Ro...	298.21 ... 298.23	98.26 ... 3174.54	ELDAR
11	vapor-liquid equilibriu...	30	1995	Lai,J.T.W.;Lau,F.W.;Ro...	296.08 ... 296.09	91.19 ... 2766.44	ELDAR
12	vapor-liquid equilibriu...	11	1995	Qian,X.;Han,B.;Liu,Y.;Y...	288.15	84.00 ... 1553.00	ELDAR
13	vapor-liquid equilibriu...	33	1995	Qian,X.;Han,B.;Liu,Y.;Y...	293.15 ... 303.15	134.00 ... 3979.00	ELDAR
14	Isothermal VLE-data (...)	42	1966	Doering,K.E.;Preuss,H.	313.15 ... 353.15	266.64 ... 47329.45	DDB-VLE
15	Isothermal VLE-data (...)	7	1998	Trandum,C.;Westh,P.;...	298.10	1203.90 ... 3161.07	DDB-VLE

Display Plot

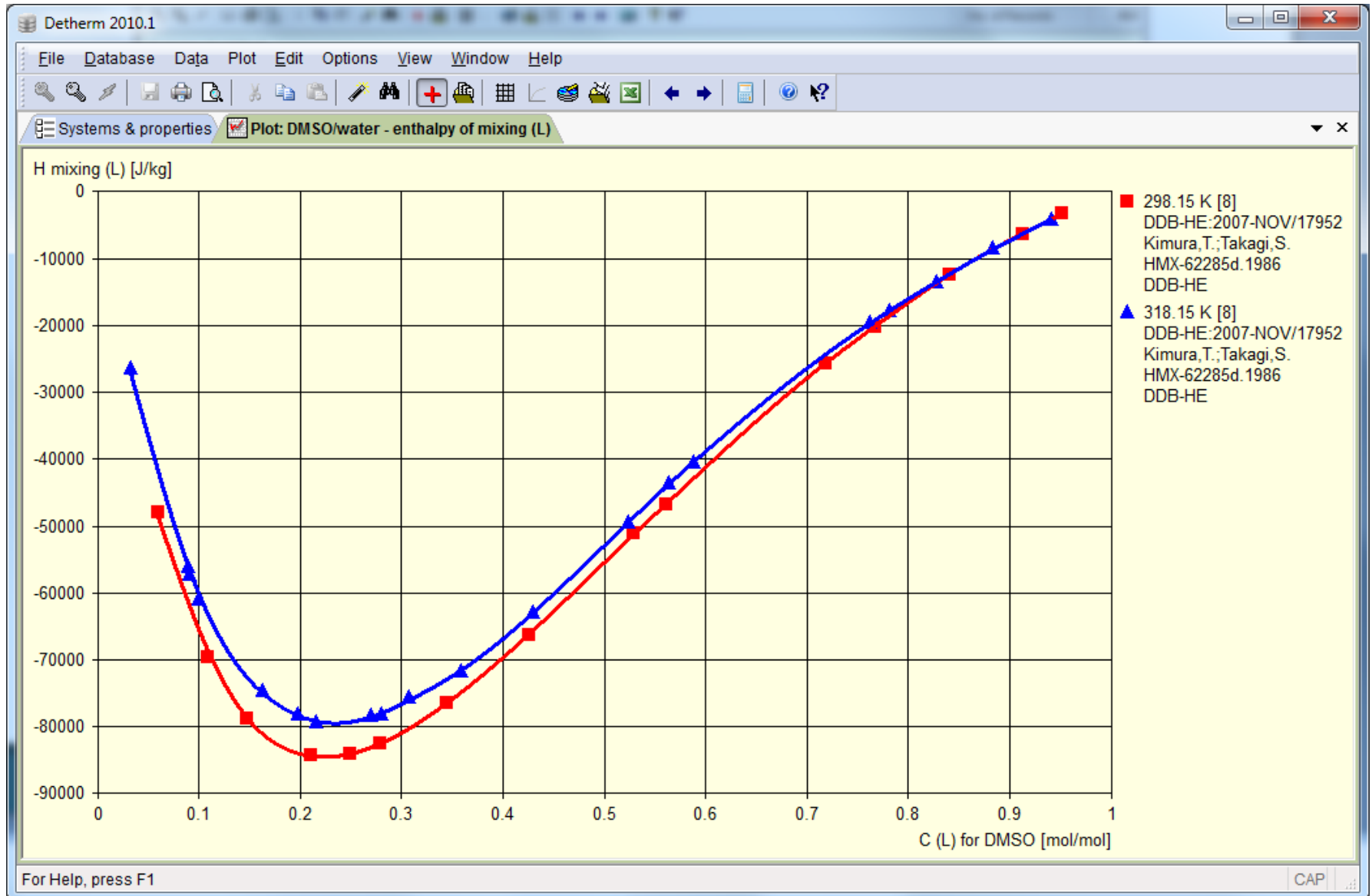
For Help, press F1

CAP

Detail plot: VLE of DMSO/water at 25 Celsius



Heats of Mixing: DMSO/Water



Pure component data of Tetrahydrofuran (THF): Vapor pressure

Detherm 2010.1

File Database Data Edit Options Ansicht Window Help

Systems & properties Plot: THF - vapor pressure

Pure components

- DMSO
- THF
 - 2nd virial coefficient (G)
 - acentric factor
 - autoignition temperature
 - boiling temperature
 - boiling temperature (L)
 - complex permittivity, imaginary part (L)
 - complex permittivity, real part (L)
 - critical compressibility factor
 - critical density
 - critical pressure
 - critical temperature
 - critical volume
 - cubic expansion coefficient (L)
 - density (L)
 - density (S)
 - dielectric constant
 - dielectric constant (L)
 - diffusion coefficient (G)
 - diffusion coefficient (L)
 - dipole moment
 - dipole moment (L)
 - enthalpy (G)
 - enthalpy (L)
 - enthalpy (related to 0 K) (G)
 - enthalpy (related to 0 K) (L)
 - enthalpy (related to 0 K) (S)

THF: vapor pressure

No.	Property	C...	Year	Author(s)	temperature [K]	p..	Data collec...
83	vapor pressure, enthalpy...	3	1981	Hossenlopp,I.A.;Scott,D.W.	301.80 ... 339.10		INFOTHERM
84	vapor pressure, density	1	1986	Anantaraman,A.V.	278.15		INFOTHERM
85	vapor pressure, viscosity...	1	1986	Anantaraman,A.V.	278.15		INFOTHERM
86	vapor pressure	13	1990	Vasil'eva,I.I.;Naumova,A...	293.15 ... 533.15		INFOTHERM
87	vapor pressure	4	1984	Jain,D.V.S.;Sidhu,R.S.	303.15 ... 323.15		COMDOR
88	vapor pressure	7	1970	Koizumi,E.;Ouchi,S.	273.50 ... 308.15		COMDOR
89	vapor pressure	1	1995	Liessmann,G.;Schmidt,...	263.15 ... 541.15		BDBB
90		27	1985		253.50 ... 361.71		DIPPR
91	vapor pressure	1	2001	Loras,S.;Aucejo,A.;Monto...	290.25 ... 338.95		INFOTHERM
92	boiling temperature, vap...	7	2004	Kao,C.P.C.;Sievert,A.C.;S...	303.04 ... 318.10		INFOTHERM
93	vapor pressure	1	2003	Segura,H.;Mejia,A.;Reich...	309.50 ... 339.10		INFOTHERM
94	vapor pressure	3	1984	Brunner,E.;Scholz,G.R.	301.55 ... 338.75		COMDOR
95	vapor pressure	3	1985	Brunner,E.	298.15 ... 373.15		COMDOR
96	vapor pressure	6	1951	Flom,D.G.;Alpert,N.;Elvin...	288.15 ... 338.15		COMDOR
97	vapor pressure	15	1970	Scott,D.W.	296.29 ... 372.85		COMDOR
98	vapor pressure	2	1988	Pividal,K.A.;Sandler,S.I.	313.15 ... 333.15		COMDOR
99	vapor pressure	4	1980	Yoshikawa,Y.;Takagi,A.;K...	338.05 ... 338.45		COMDOR
100		3			283.15 ... 313.15		DIPPR
101		15	1973	Boublik,T.;Fried,V.;Hala,E.	296.29 ... 372.85		DIPPR
102		27	1956	Kobe,A.K.;Ravicz,A.E.;Vo...	394.26 ... 538.71		DIPPR
103		25	1984	Kudchadker,A.P.;Kudcha...	253.15 ... 540.15		DIPPR
104		1	2008	DIPPR	164.65 ... 540.15		DIPPR

Display Plot

For Help, press F1

CAP

Vapor pressure of THF: Plot of some data sets

