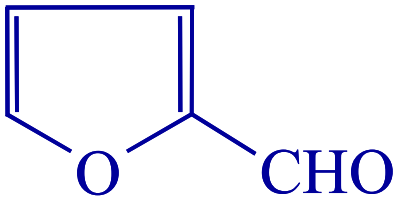
BIOMASS BASED CHEMICALS

PHYSICAL PROPERTIES OF FURFURAL



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1. OVERVIEW:

1.1 GENERAL PROPERTIES:

Molecular weight	**96.08**
Boiling point at 101.3 kPa (1 atm), °C	**161.7**
Freezing point, °C	**-36.5**
Refractive index, n_D	
20°C	**1.5261**
25°C	**1.5235**
Density, d_4 at 20°C, g/cm^3	**1.1598**
Vapor density (air=1)	**3.3**
Critical pressure, P_c, MPa	**5.502**
Critical temperature, T_c, °C	**397**
Solubility in, wt%	
water	**8.3**
alcohol; ether	∞

1.2 THERMODYNAMIC PROPERTIES:

Heat of vaporization (liq), kJ/mol	42.8
Heat capacity (liq), J/(g.K)	
20-100°C	1.74
Heat of combustion (liq), kJ/mol	2344
Enthalpy of formation, kJ/mol	-151

1.3 FLUID PROPERTIES:

Viscosity, mPa.s, 25°C	1.49
Surface tension, mN/m (=dyn/cm)	
29.9°C	40.7

1.4 ELECTRICAL PROPERTIES:

Dielectric constant 20°C	41.9

1.5 FLAMMABILITY PROPERTIES:

Explosion limits (in air), vol%	2.1-19.3
Flash point, °C, tag closed cup	61.7
Auto ignition temperature, °C	315

2. PHYSICAL PROPERTIES IN DETAIL:

2.1 VAPOR PRESSURE:

$$p_i = \exp(a + b/T + c.\ln(T) + d.T^2)$$

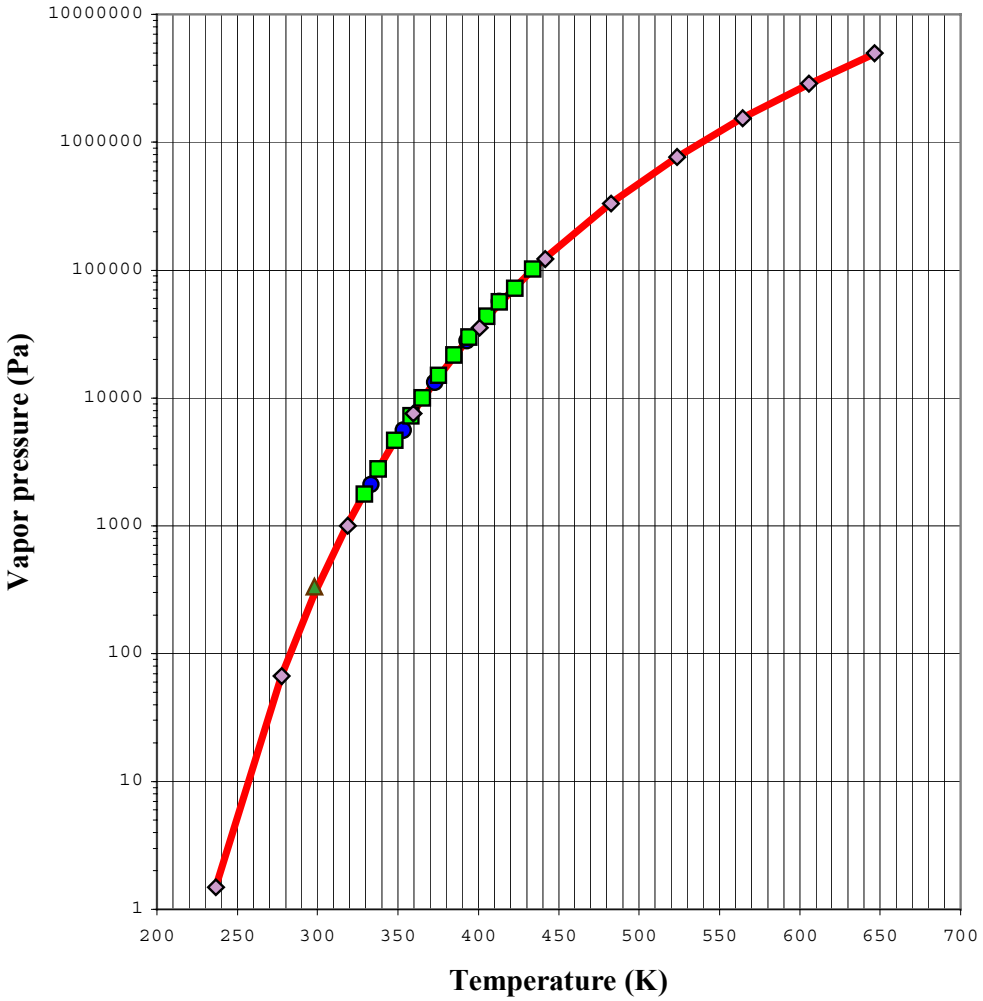
a = *78,653*

b = *-8043*

c = *-8,1424*

d = *4,509e-6*

(p_i in Pa; T in K)



▲ Experimental data from Riddick, J.A., Bunger, W.B., "Organic Solvents: Physical Properties and methods of purification," 3rd ed. Wiley Interscience, New York (1970)

● Experimental data from Kirk-Othmer, " Encyclopedia of Chemical Technology," 3rd ed., Interscience, New York (1978)

■ Experimental data from Matthews, J.B., Sumner, J.F., Moelwyn-Hughes, E.A., "The vapor Pressures of Certain Liquids,' Trans. Faraday Soc. 46, 797 (1950).

◆ Predicted data from Othmer, D.F., Yu, E. "Correlating Vapor pressures an Vapor Volumes,' Ind.Eng. Chem. 60,22 (1968)

2.2 THERMAL CONDUCTIVITY:

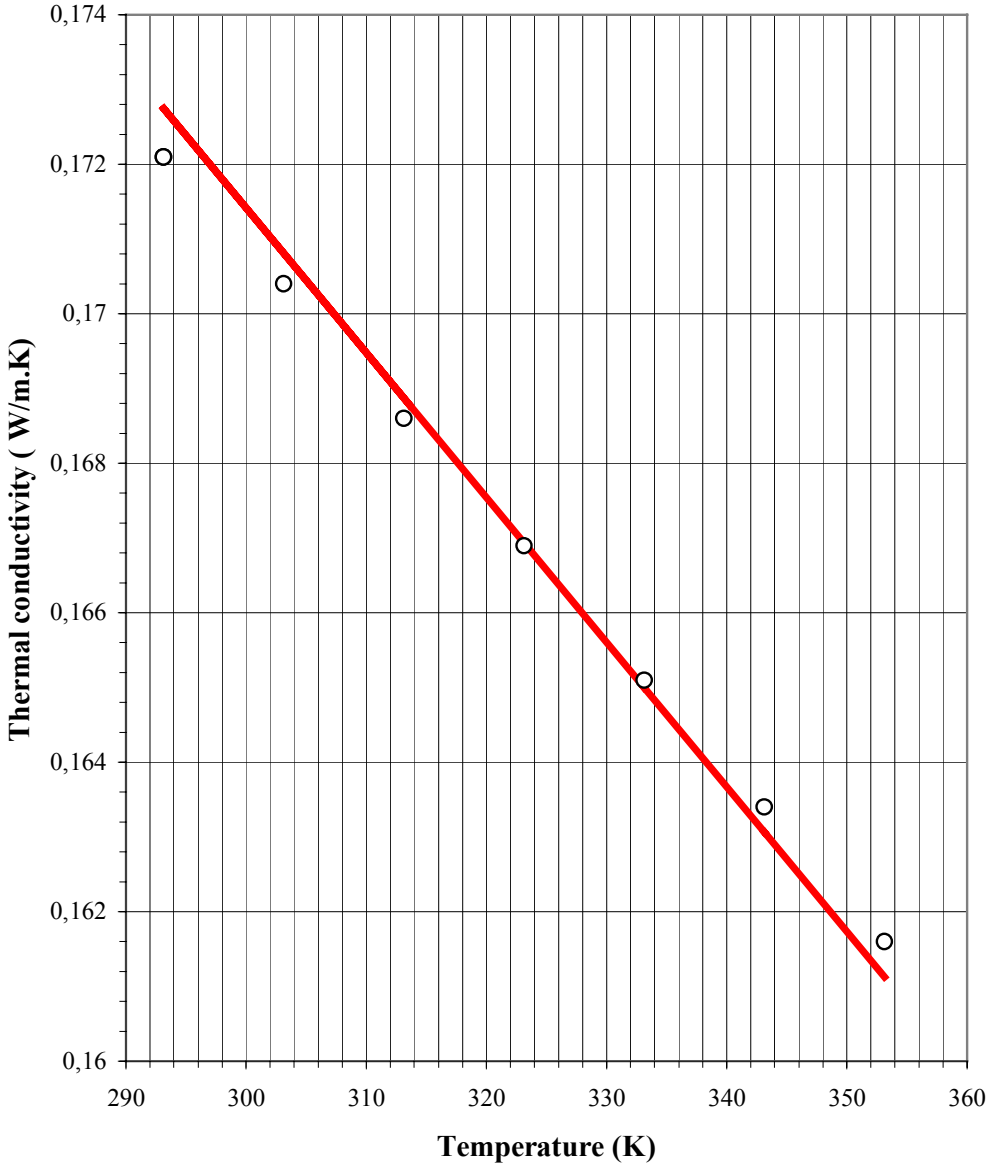
Liquid

$\lambda = a + b.T$

$a = 0,2295$

$b = -1,936e-4$

(λ in W/m.K ; T in K)



○ Experimental data from Geller, Z.I., Rastroguev, Yu.L., Ganiev, Yu.A., "Thermal Conductivity of Selected solvents," Izv. Vyssh. Ucheb. Zaved., Neft Gaz 8(6), 79 (1965)

Vapor

$\lambda = (a.T^b)/(1 + c/T + d/T^2)$

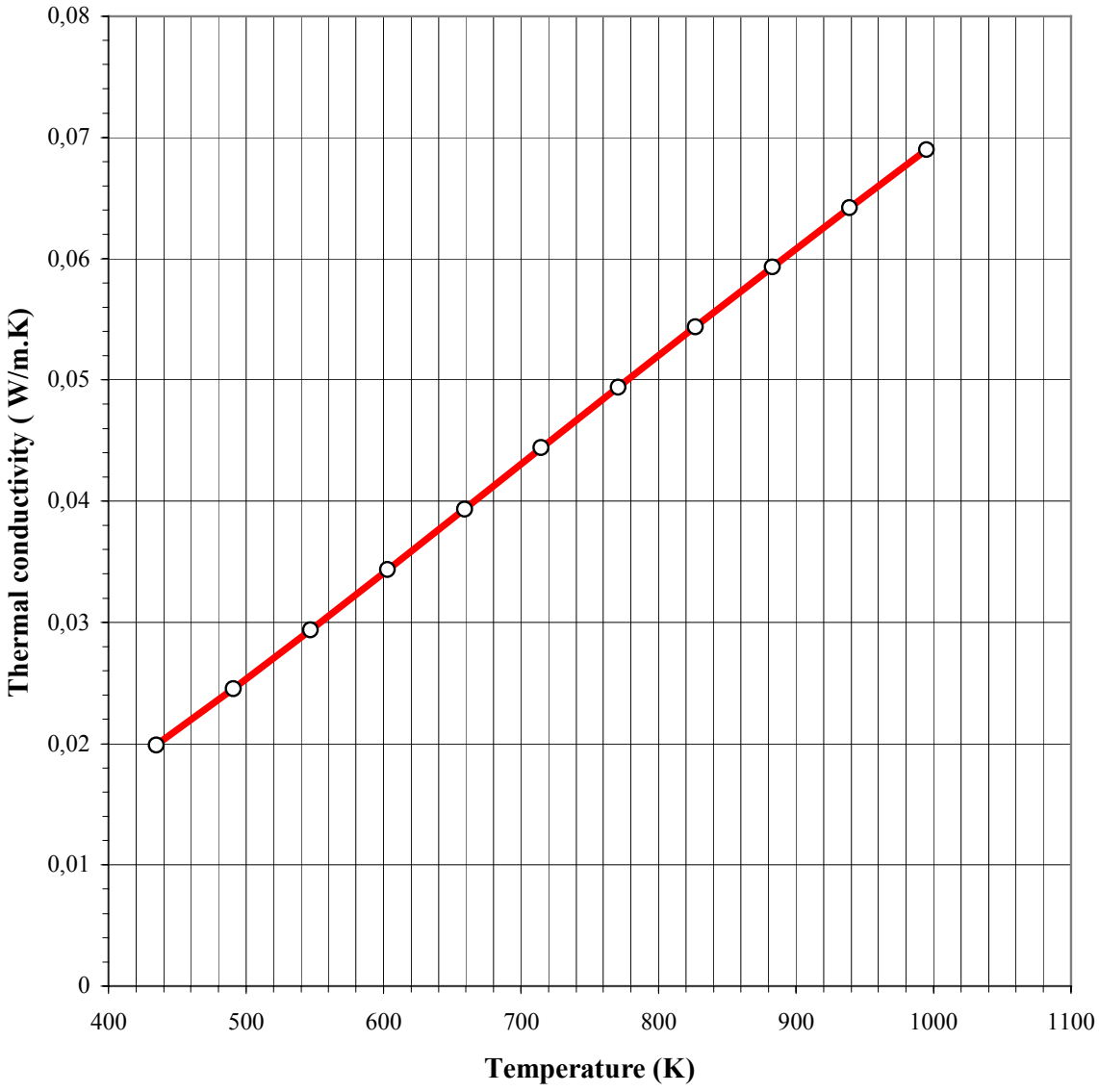
a = 8,3221e-3

b =0,4228

c = 637,87

d = 5,502e5

(λ in W/m.K ; T in K)



O Predicted data from Stiel, L.I., Thodos, G.,"The thermal conductivity of nonpolar substances in the dense gaseous and liquid regions," AIChe J. 10, 266 (1964)

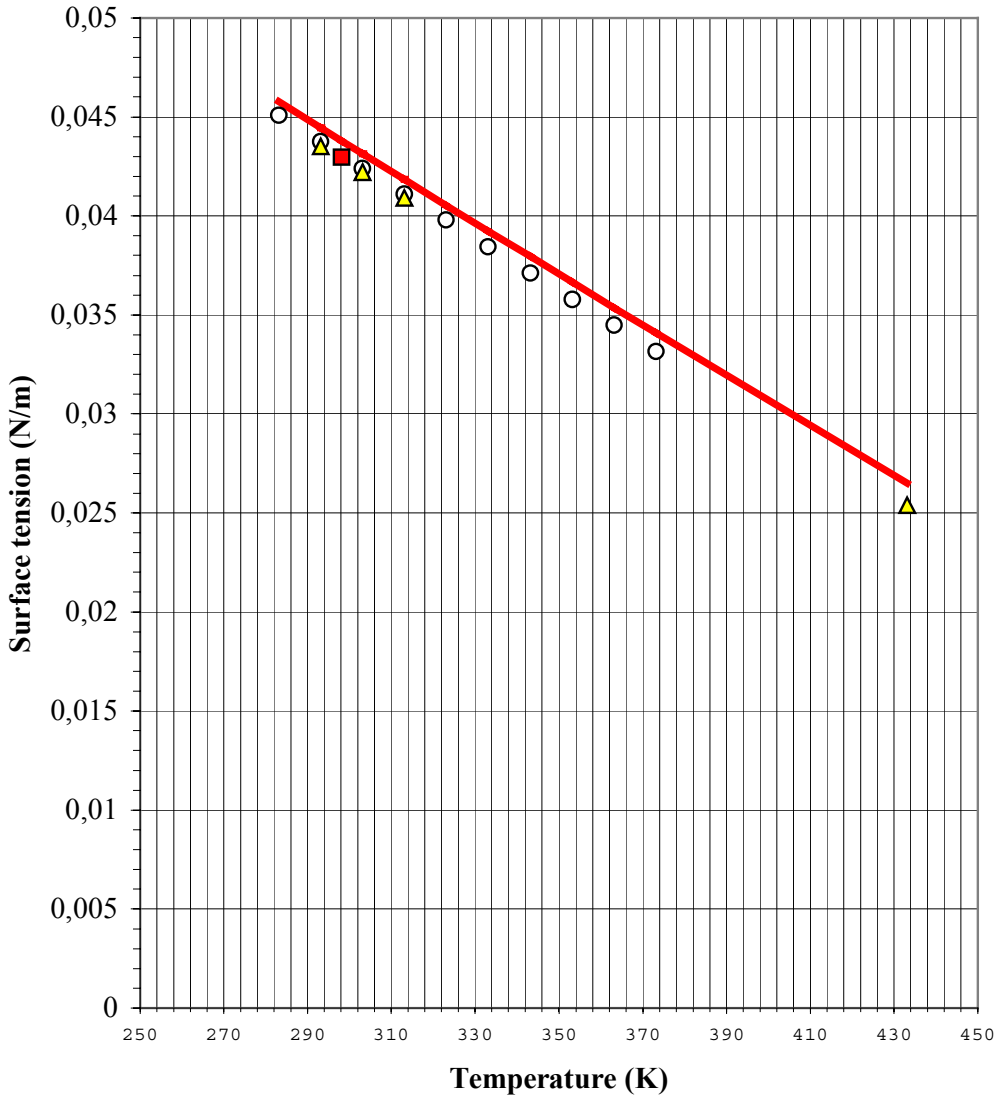
2.3 SURFACE TENSION:

$$\sigma = a.(1 - T_r)^b$$

$a = 0{,}08429$

$b = 1{,}1124$

(σ in N/m ; T in K)



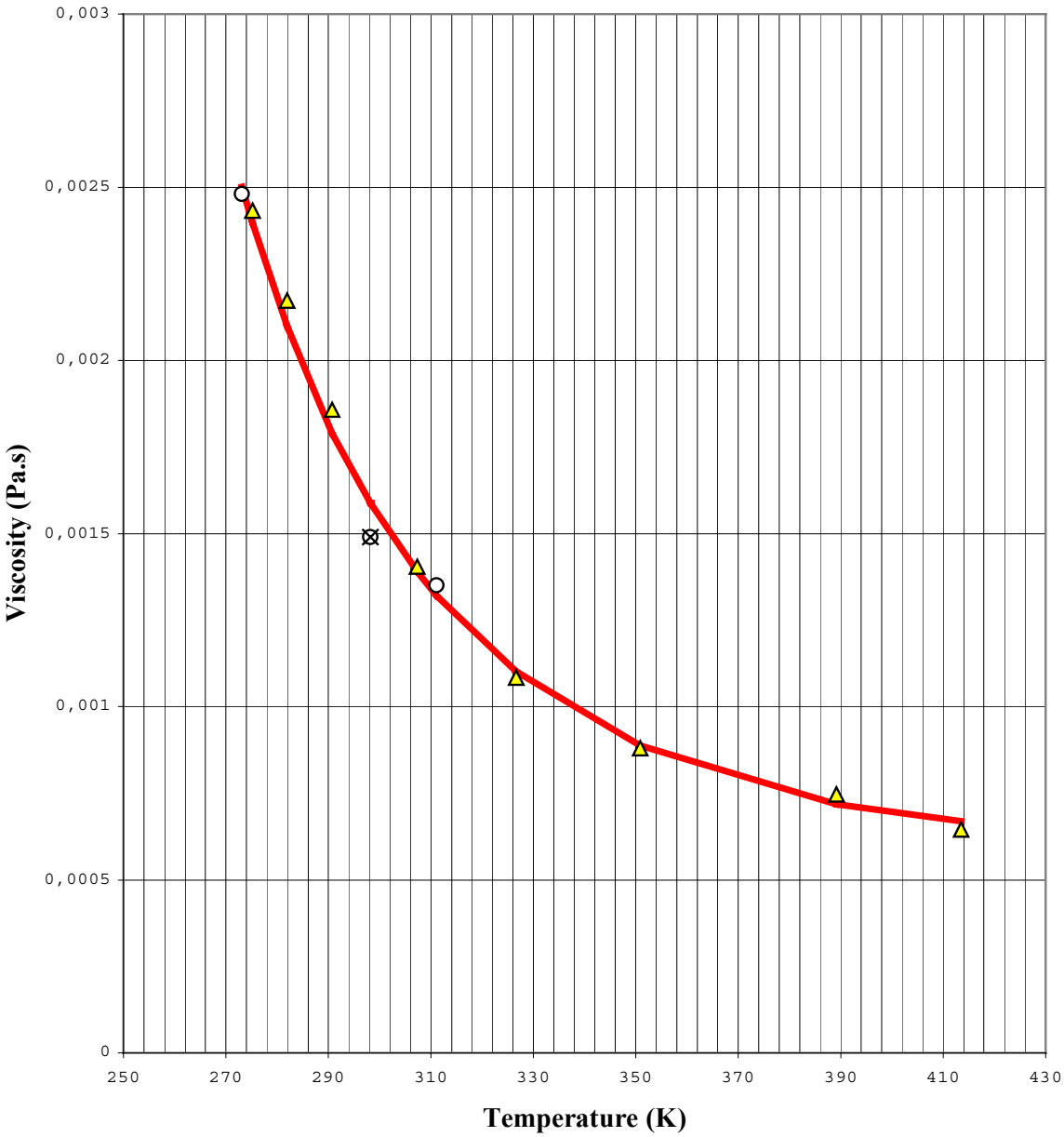
○ Data from Jasper, J.J., "The surface Tension of Pure Liquid compounds,"J. Phys. Chem. Ref. Data 1(4), 841 (1972)

△ Data from International Critical Tables of Numerical Data, Physics, Chemistry, and Technology (7 vols. + Index), edited by E.W. Washburn, McGraw-Hill, New York (1926-1933)

■ Data from Murphy, N.F., Lastovica, J.E., Fallis, J.G., "Correlation of Interfacial Tension of Two-Phase, Three-Component Systems," Ind. Eng. Cehm. 49(6), 1035 (1957)

2.4 VISCOSITY:

Liquid
$\mu = \exp(a + b/T + c.\ln(T))$
a = *-69,008*
b = *3950,4*
c = *8,655*
(m in Pa.s ; T in K)

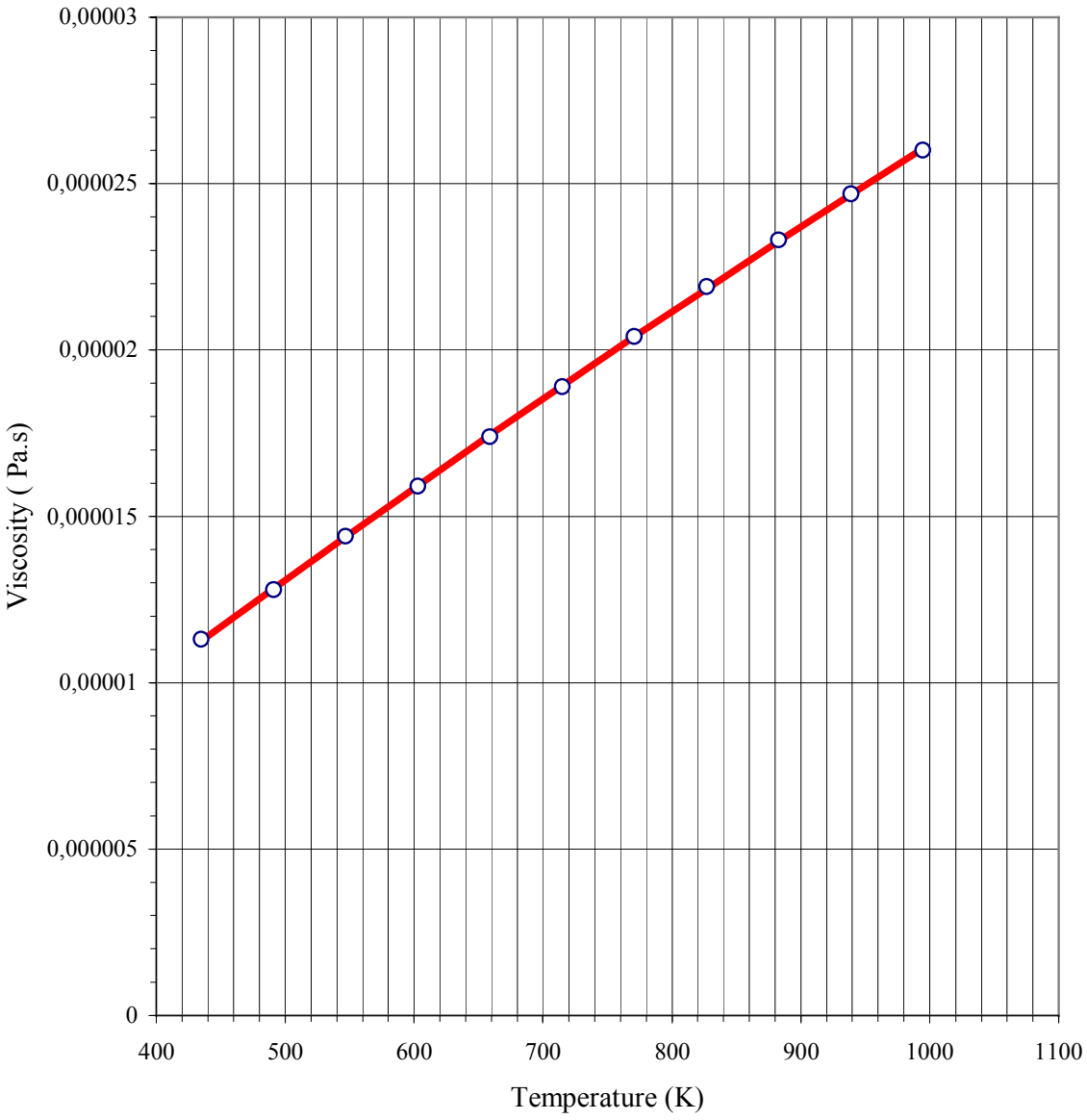


○ Experimental data from Riddick, J.A., Bunger, W;B., "Organic Solvents : Physical Properties and Methods of purification, "3rd ed., Wiley Interscience, New york (1970)

△ Predicted data from Gallant, R.W., "Physical Properties of Hydrocarbons," Gulf Publishing Co?, Houston, Texas (Vol.1,1968; Vol.2 1970)

✕ Experimental data from Kirk-Othmer, "Encyclopedia of Chemical Technology," 3rd ed., Interscience, New york (1978)

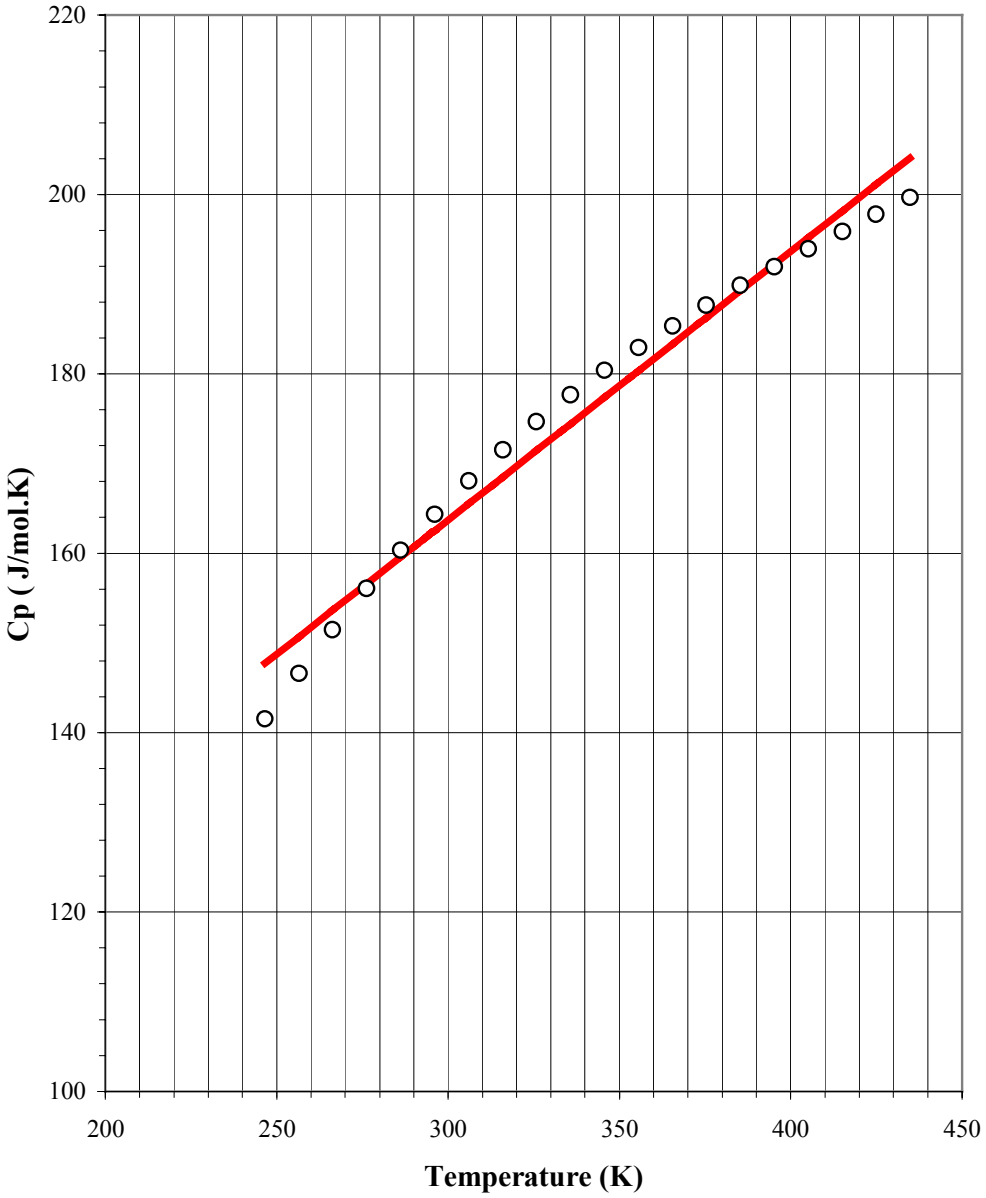
Vapor
$\mu = (a.T^b)/(1 + c/T)$
a = 1,7834e-7
b = 0,7524
c = 231,09
(μ in Pa.s ; T in K)



Predicted data from Chapman, S., Cowling, T.G., "The Mathematical Theory of Non-uniform gases," Cambridge University Press, Cambridge, England (1952) and Stiel, L.T., Thodos, G., "Force Constants for Polar Substances : their prediction from critical Prope

2.5 HEAT CAPACITY AT CONSTANT PRESSURE:

Liquid
cp = a + b.T
a *= 73,9*
b *= 0,2994*
(cp in J/mol.K ; T in K)



○ Predicted data from Lee, B.I., Kesler, M.G., " A generalised Thermodynamic Correlation Based on Three Parameter Corresponding States," AIChe J. 21(3), 510 (1975)

Vapor

$$cp = a + b.((c/T)/\sinh(c/T))^2 + d.((e/T)/\cosh(e/T))^2$$

a = 47,3

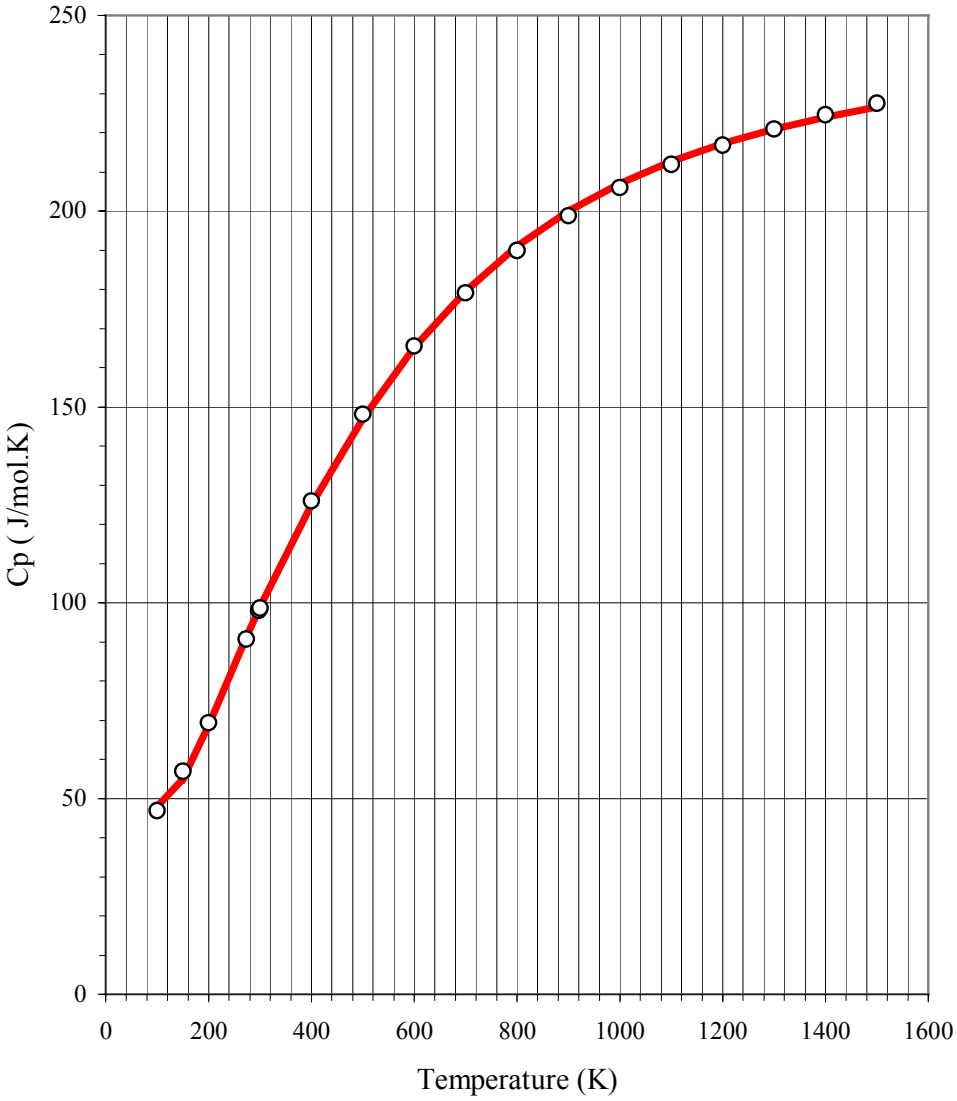
b = 198,3

c = 1040,6

d = 109

e = 472,6

(cp in J/mol.K ; T in K)



○ Predicted data from Kudchadker, S.A. Kudchadker, A.P., "Thermodynamic Properties of Oxygen Compounds. III. Benzaldehyde and Furfural (2-Furaldehyde)," Thermochim. Acta 12,432 (1975)

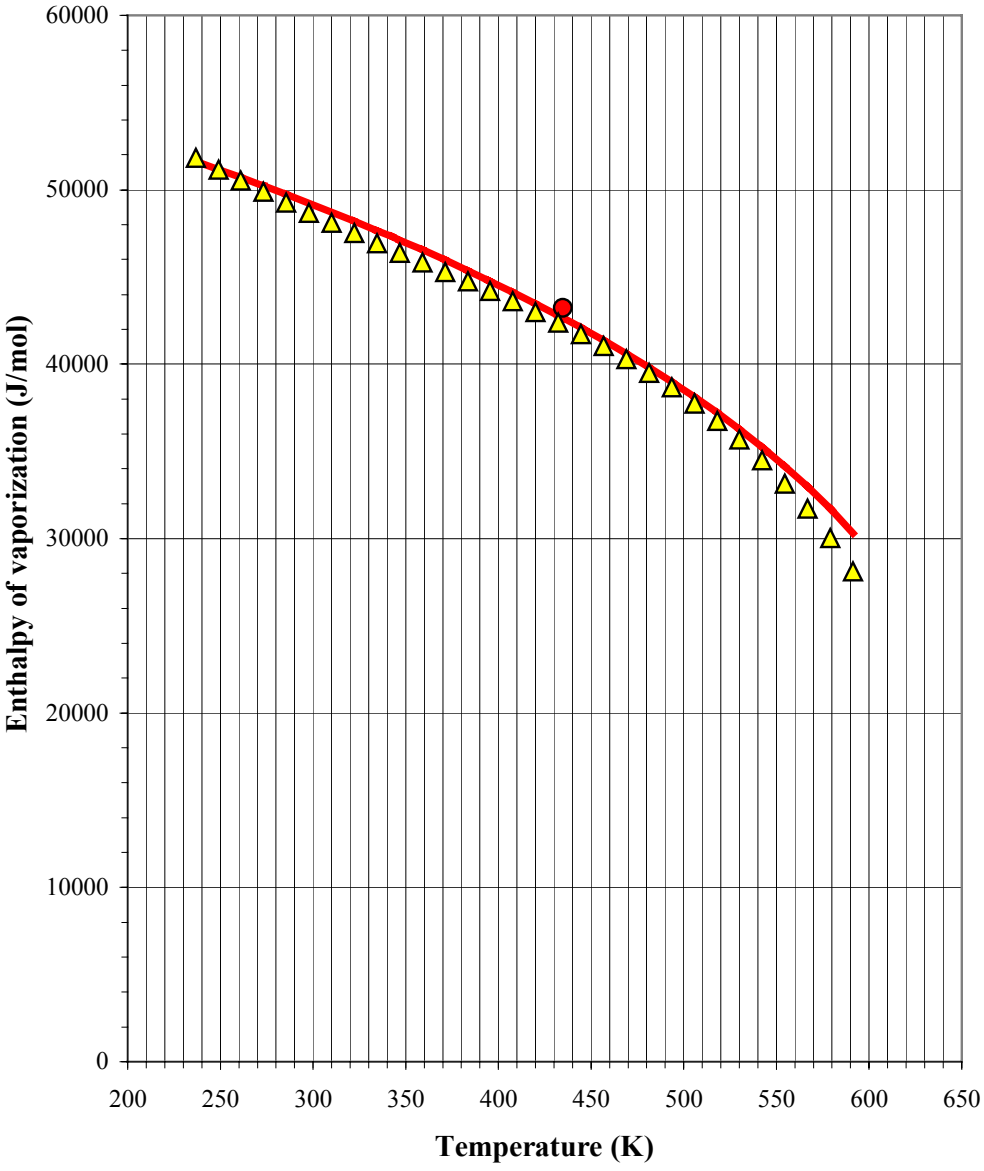
2.6 ENTHALPY OF VAPORIZATION:

$$\Delta H_{vap} = a.(1- Tr)^{b}$$

$$a = 59610$$

$$b = 0,3126$$

(ΔH_{vap} in J/mol ; T in K)

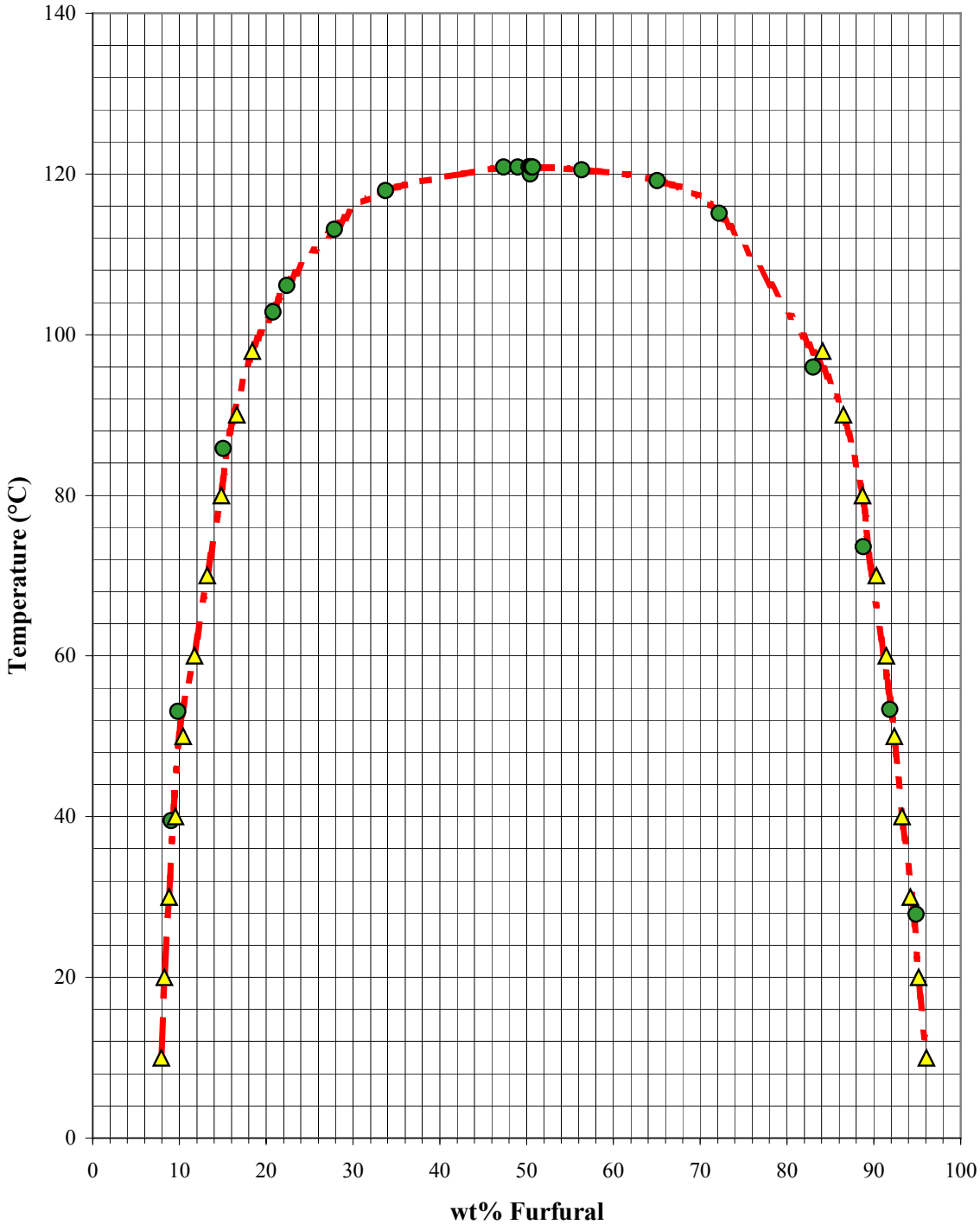


● Data from Riddick, J.A., Bunger, W;B. "Organic solvents : Physical Properties an Methods of purification," 3rd ed., wiley Interscience, New York (1970)

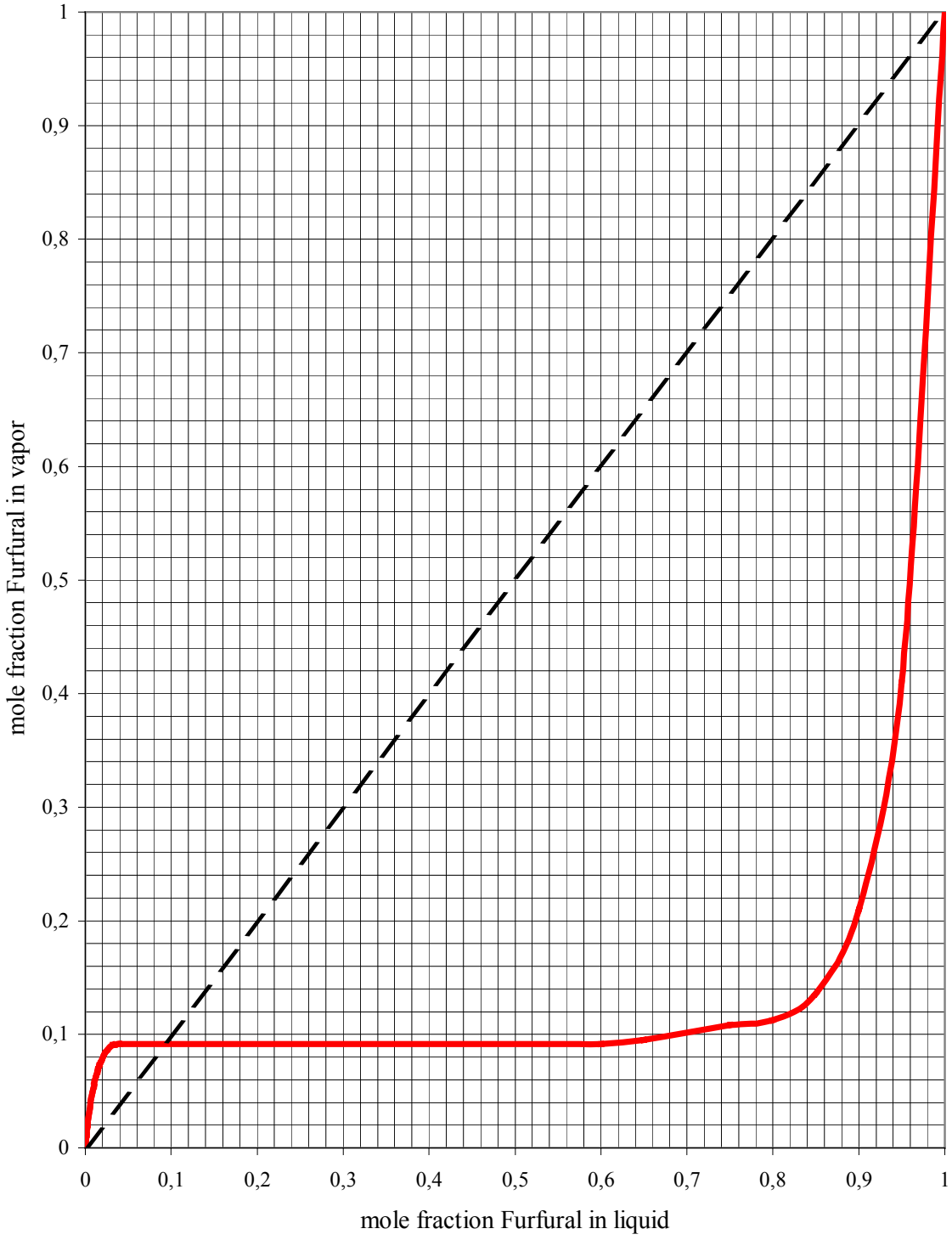
△ Data calculated from the Clapeyron Equation

2.7 FURFURAL-WATER:

Furfural-Water Solution-Temperature Diagram

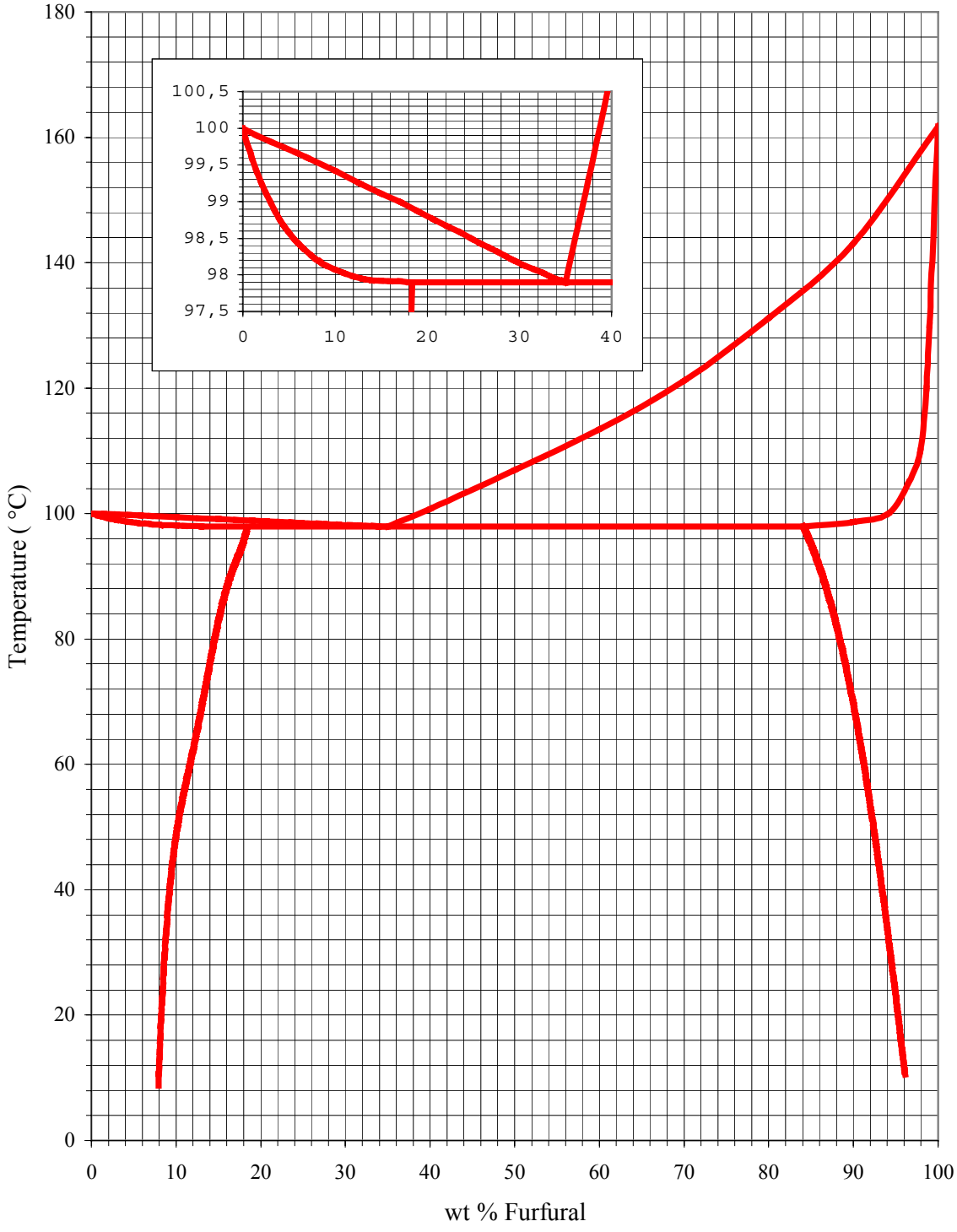


Furfural-Water
Vapor-liquid composition



Based on data from Mains, G.H., Chem. & Met. Eng.,26,779 (1922)

Furfural-Water
Vapor-liquid equilibrium



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The data contained herein are based on information currently available to us and believed to be factual and the opinions expressed to be those of qualified experts; however, these data are not to be taken as a warranty of representation for which TransFurans Chemicals assumes legal responsibility.

Physical Properties of Furfural 1^{e} version 12/22/2000