BIOMASS BASED CHEMICALS

PHYSICAL PROPERTIES OF FURFURYL ALCOHOL

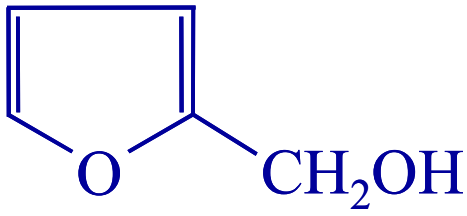


TABLE OF CONTENTS

1. OVERVIEW:

1.1 GENERAL PROPERTIES:

Molecular weight	**98.10**
Boiling point at 101.3 kPa (1 atm), °C	**170**
Freezing point, °C	
Metastable crystalline form	**-29**
Stable crystalline form	**-14.6**
Refractive index, n_D	
20°C	**1.4868**
25°C	**1.4843**
Density, d_4 at 20°C, g/cm^3	**1.1285**
Vapor pressure	
Vapor density (air=1)	**3.4**
Critical pressure, P_c, MPa	**5.35**
Critical temperature, T_c, °C	**359**
Gibb's free energy of formation	
Solubility in, wt%	
water	∞
alcohol; ether	∞

1.2 THERMODYNAMIC PROPERTIES:

Heat of vaporization (liq), kJ/mol	**50.1**
Heat capacity (liq), J/(g.K)	
25°C	**2.10**
Heat of combustion (liq), kJ/mol	**2548**
Enthalpy of formation, (kJ/mol)	**-218.9**

1.3 FLUID PROPERTIES:

Viscosity, mPa.s, 25°C	**4.62**
Surface tension, mN/m (=dyn/cm)	
25°C	**38.2**

1.4 FLAMMABILITY PROPERTIES:

Explosion limits (in air), vol%	**1.8-16.3**
Flash point, °C, tag closed cup	**65**
Auto ignition temperature, °C	**391**

2. PHYSICAL PROPERTIES IN DETAIL:

2.1 VAPOR PRESSURE:

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

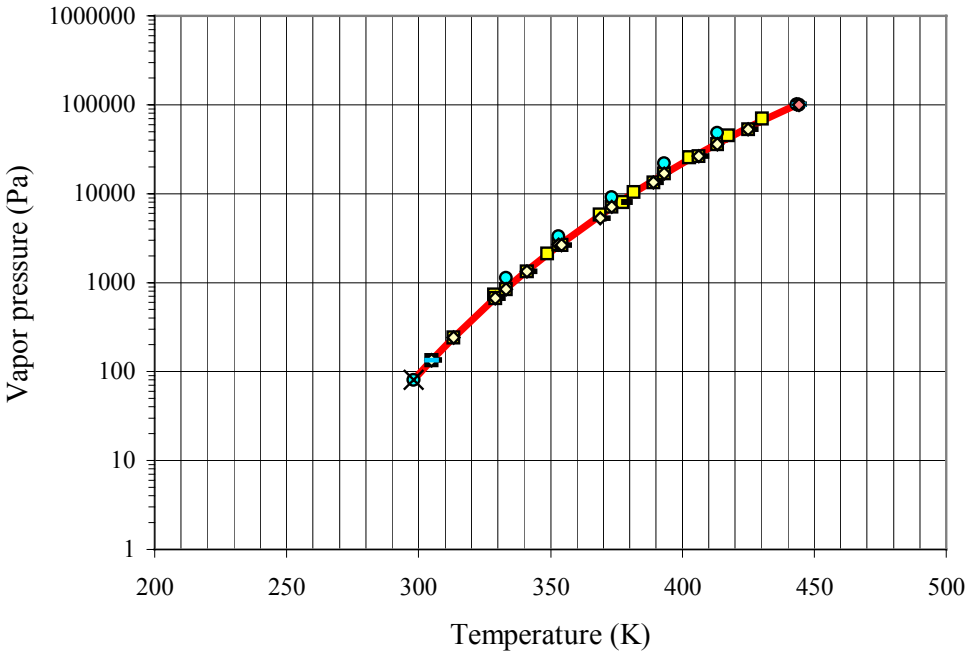
a = 77,274

b = -8715,5

c = -7,9113

d = 4,7922 e-3

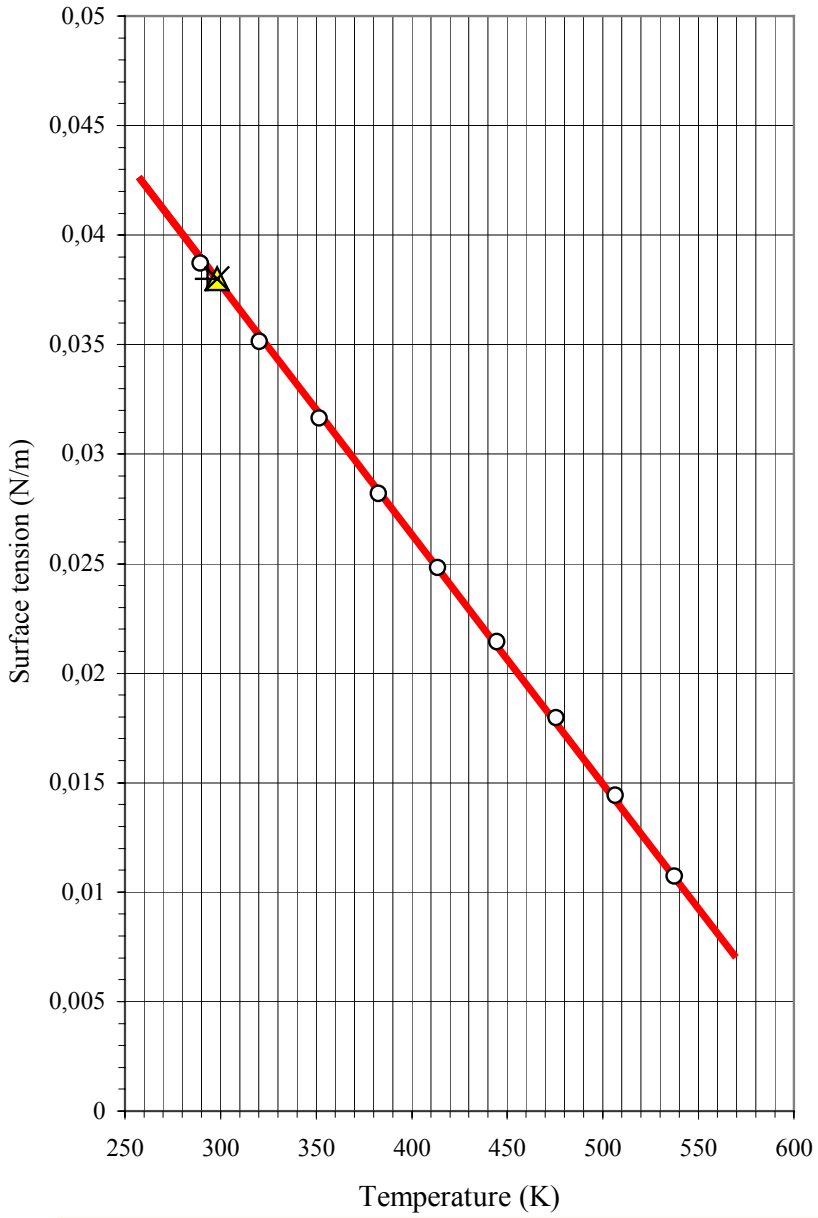
(p_i in Pa; T in K)



- Experimental data from The Quaker Oats company," Qo Furfuryl alcohol," Bulletin 205-B, Chicago, IL
- Experimental data from Kirk-Othmer,"Encyclopedia of Chemical Technology," 3rd ed., Interscience, New york
- Experimental data from Riddick, J.A., Bunger, W.B., "Organic solvents : Physical Properties and Methods of Purification, "3rd ed., Wiley Interscience, New Yrok (1970)
- Experimental data from Sax, N.I., "Dangerous Properties of Industrial Materials," 6th ed., Van Nostrand Reinhold Company, New York (1984)
- Experimental data from Stull, D.R., "Vapor Pressure of Pure Substances," Ind. Eng. Chem. 39,517 (1947)
- Experimental data from Dunlop, A.P., Peters, F.N., " The Furans," Reinhold, New york (1953)
- Experimental data from Handbook of Laboratory Safety, 2nd Ed., Edited by Norman V. Steere, CRC Press Inc. Boca Raton, FL (1982)
- Experimental data from Handbook of Data on Organic Compounds, edited by R.C. Weast, M.J. Astle, CRC Press, Inc. Boca Raton, FL (1985)

2.2 SURFACE TENSION:

$\sigma = a.(1 - T_r)^b$
a = 0,07217
b = 1,006
(σ in N/m ; T in K)



○ Predicted data from Sugden, S., "The Variation of Surface Tension with Temerature and some related Functions," J. Chem. Soc. (London, Transactions) 125, 32 (1924)

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

× 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 Weiss, G. (editor), "Hazardous Chemicals Data Book," Noyes Data Corporation, Park Ridge, New Jersey (1980)

2.3 VISCOSITY:

Liquid

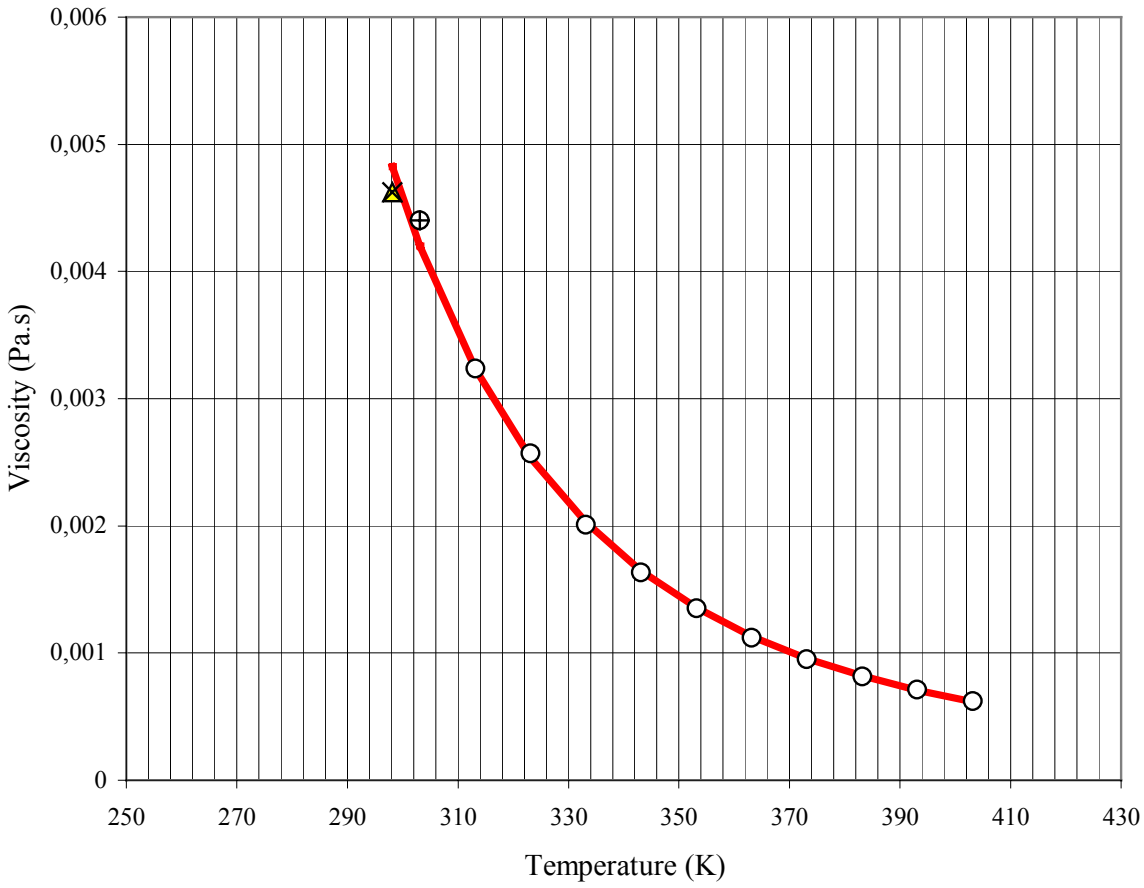
$\mu = \exp(a + b.T + c.T^{2)}$

a = -37,008

b = 3555

c = 3,4664

(μ in Pa.s ; T in K)



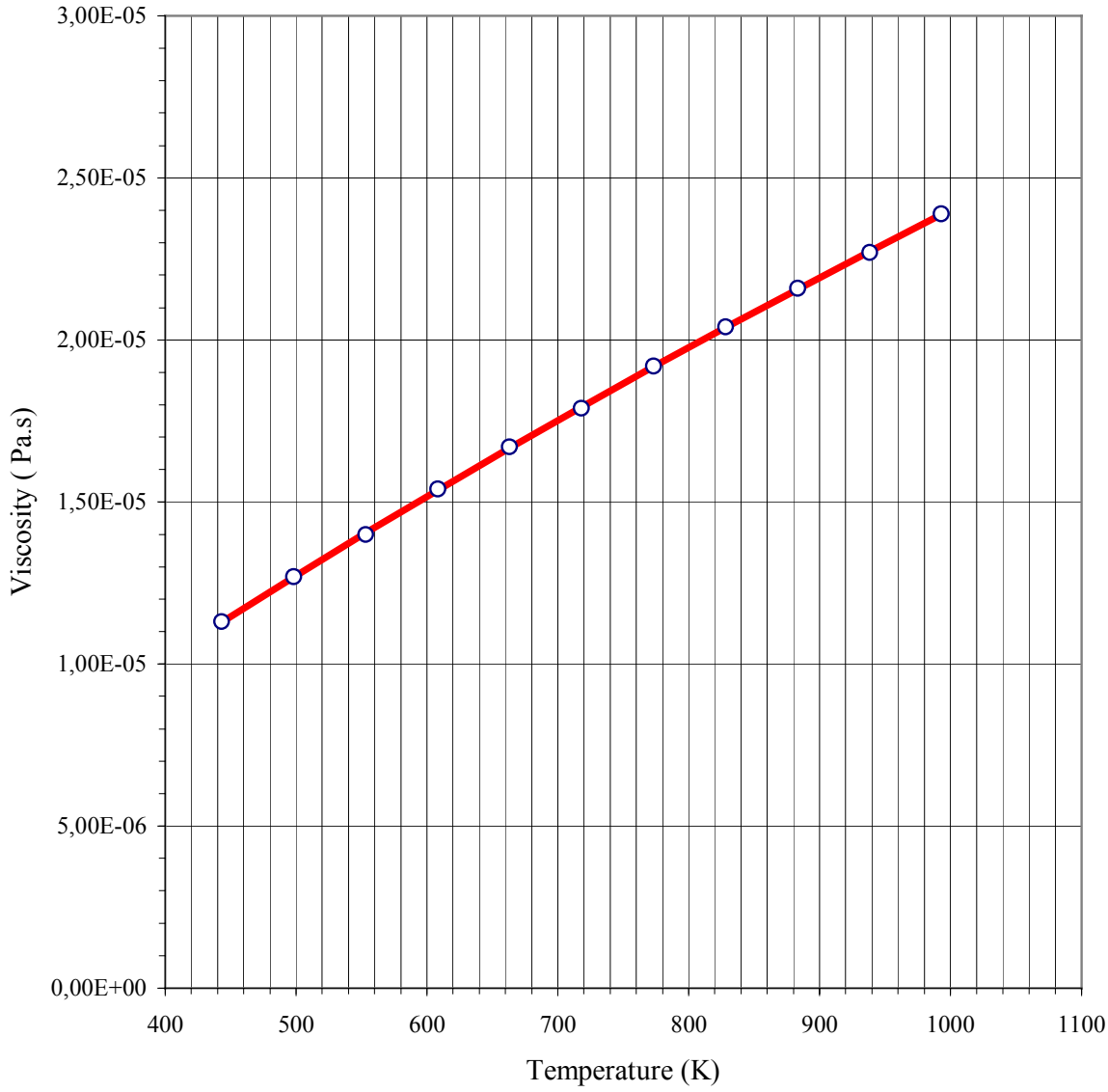
○ Experimental data from Mason, D.M., wilcox, O.W., Sage, B.H., "Viscosities of Several Liquidq," J.Phys.Chem. 56, 1008 (1952)

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

× Experimental data from Riddick, .A. Bunger, W.B., "Organic Solvents : Physical Properties and Methods of Purification," 3rd ed., Wiley Interscience, New York (1978)

+ Experimental data from Dudzik, Z. Glowinkowski, s. Pajak, Z. Szuba, Z., "Nuclear Magnetic Relaxation in the polycondensation Processes of Furfuryl Alcohol," Bull. Acad. Pol.Sci, Ser. Sci. Chim 22 (9), 759 (1974)

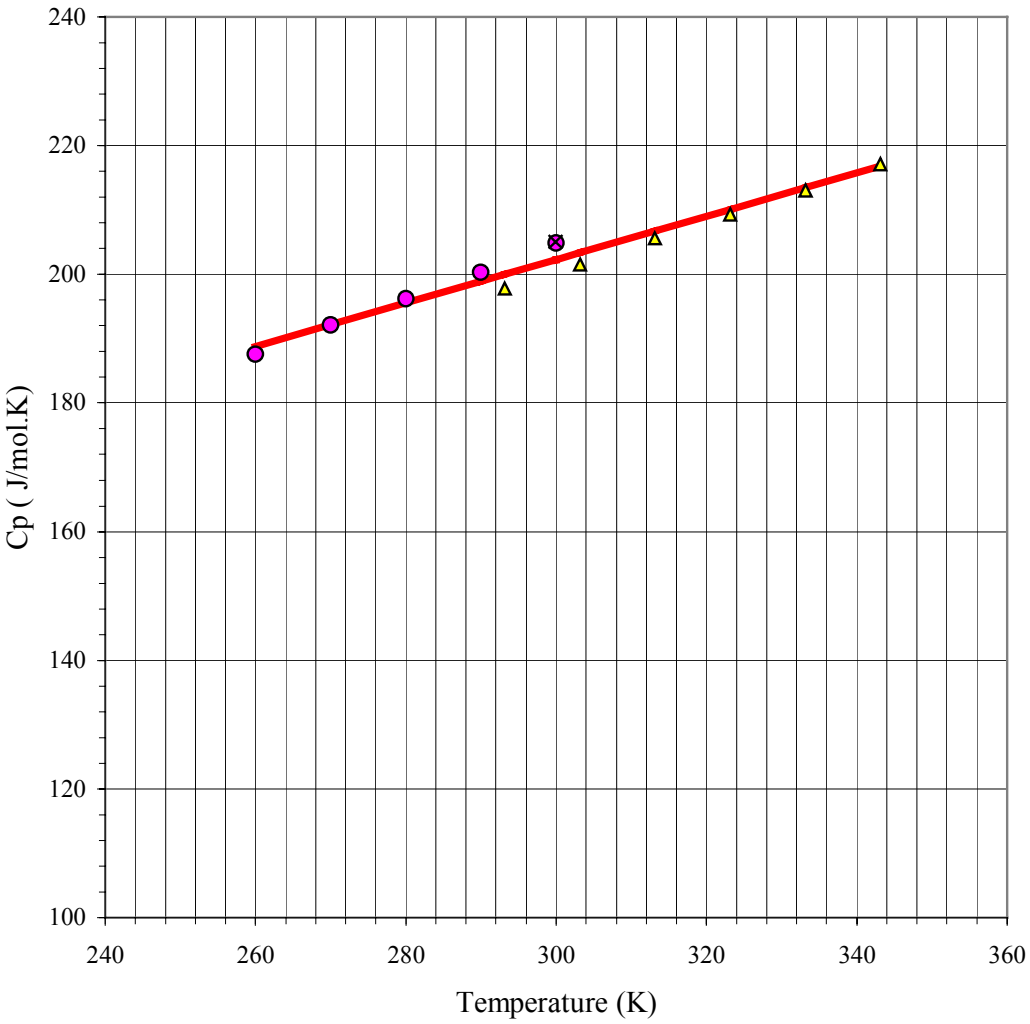
Vapor
$\mu = (a.T^b)/(1+c/T)$
a = 2,9819 e-7
b = 0,6658
c = 233,43
(μ in Pa.s ; T in K)



Predicted data from Reichenberg, D "The viscosity of Organic Vapors at Low Pressures," DSC Rep. 11, National Physical Laboratory, Teddington, England August 1971

2.4 HEAT CAPACITY AT CONSTANT PRESSURE:

Liquid
Cp = a + b.T
a =101,2 ; b = 0,337
(Cp in J/mol.K ; T in K)

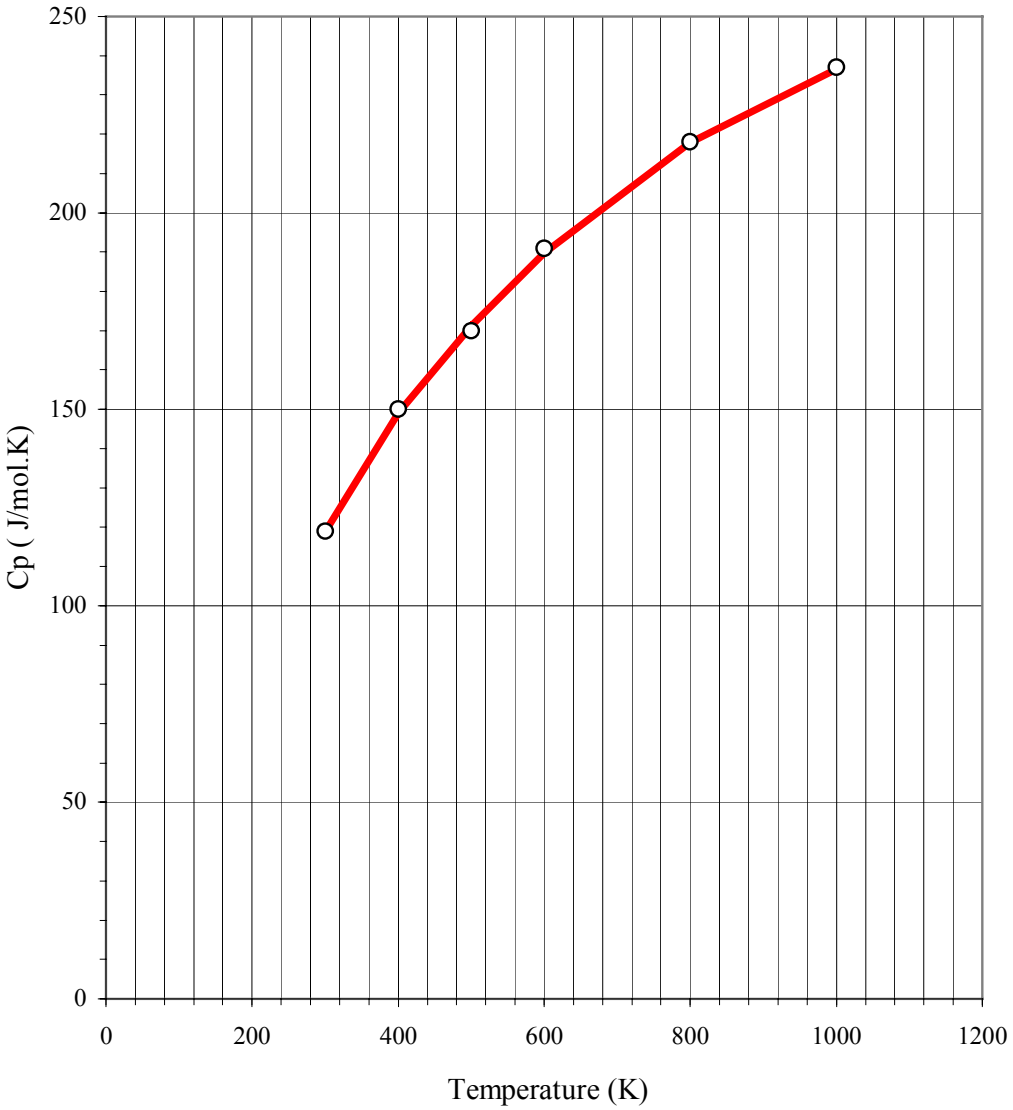


- Experimental data from Parks, G.S., Kennedy, W.D., Gates, R.R., Moore, G.E., Renquist, M.L., "Thermal Data on Organic Compounds. XXVI. Some heat capacity, Entropy and Free energy Data for seven compounds containing Oxygen," J.Am. Chem. Soc. 78 , 56 (1956)
- Experimental data from Hough, E.W., mason, D.M. Sage, B.H., "Heat capacities of Several Organic liquids," J.Amer.Chem.Soc. 72;5775 (1950)
- Experimental data from Riddick, J.A., Bunger, W.B.,"Organic solvents : Physical properties and Methods of purification," 3rd ed., wiley Interscience", New York (1970)

Vapor

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

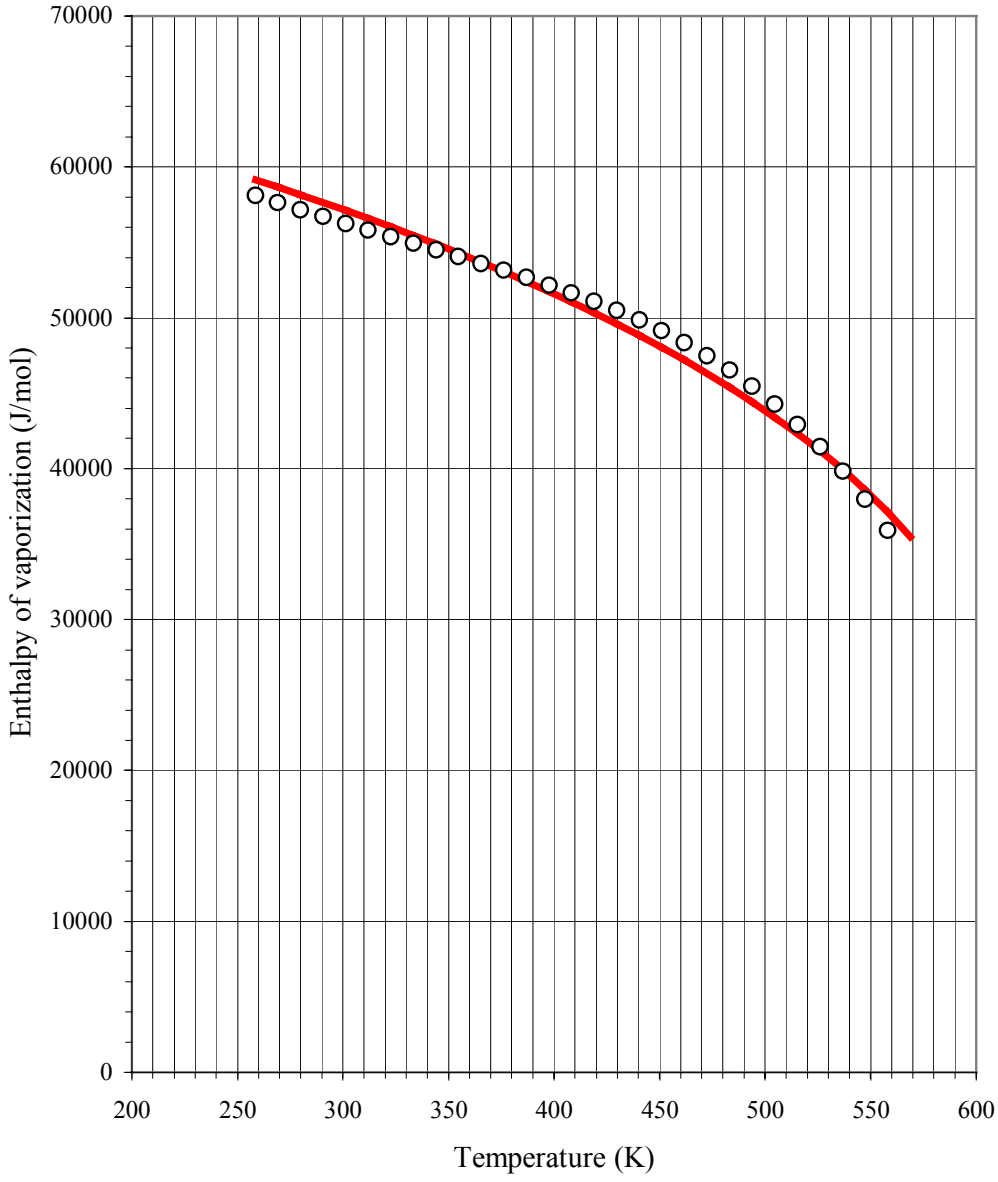
a = 169,17;
b = 117,3;
c = 1229
d = -78470
e = 7,742
(cp in J/mol.K; T in K)



O Predicted data from Rhodes, Clyde L., II, " A computer Algorithm to perform Chemical Structure analysis for Group contribution calculations," M.S. thesis, The Pennsylvania State University, University park, PA (1984)

2.5 ENTHALPY OF VAPORIZATION:

$\Delta H_{vap} = a.(1-T_r)^b$
a = 68820
b = 0,2876
(ΔH_{vap} in J/mol ; T in K)



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 Furfuryl Alcohol 1e version 12/22/2000