LIBRARY OF PHYSICO-CHEMICAL PROPERTY DATA

Handbook of Thermodynamic Diagrams

Volume 3

Organic Compounds C_8 to C_{28}

Carl L. Yaws

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Gulf Publishing Company
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DISCLAIMER

This handbook presents a variety of thermodynamic and physical property data. It is incumbent upon the user to exercise judgment in the use of the data. The author and publisher do not provide any guarantee, express or implied, with regard to the general or specific applicability of the data, the range of errors that may be associated with any of the data, or the appropriateness of using any of the data in any subsequent calculation, design, or decision process. The author and publisher accept no responsibility for damages, if any, suffered by any reader or user of this handbook as a result of decisions made or actions taken on information contained herein.

PREFACE

Thermodynamic property data are important in many engineering applications in the chemical processing and petroleum refining industries. The objective of this book is to provide the engineer with such data. The data are presented in thermodynamic diagrams (graphs) covering a wide range of pressures and temperatures to enable the engineer to quickly determine values at points of interest. The contents of the book are arranged in the following order: graphs, references, and appendixes.

The graphs are arranged by carbon number and chemical formula to provide ease of use. English units are used for the property values. For those involved in SI and metric usage, each graph displays a conversion factor to provide the SI and metric units.

The graphs provide wide coverage for volume and enthalpy as a function of temperature and pressure, including the following:

- two-phase region for saturated liquid and vapor
- superheated gas region for gases above saturation temperature
- subcooled liquid region for liquids below saturation temperature
- supercritical region for temperatures and pressures above critical point

The graphs for enthalpy also contain lines of constant entropy to permit engineering usage for 2nd law problems such as adiabatic expansion and compression of fluids.

The coverage encompasses a wide range of organic compounds including hydrocarbons, such as alkanes, olefins, acetylenes, and cycloalkanes; oxygenates, such as alcohols, aldehydes, ketones, acids, ethers, glycols, and anhydrides; halogenates, such as chlorinated, brominated, fluorinated, and iodinated compounds; nitrogenates, such as nitriles, amines, cyanates, and amides; sulfur compounds, such as mercaptans, sulfides, and sulfates; silicon compounds, such as silanes and chlorosilanes; and many other chemical types.

The range of coverage for pressure is from 10 to 10,000 psia. Very limited experimental data are available at pressures above 1,000 to 2,000 psia. Thus, values at the higher pressures should be considered rough approximations. Values at lower pressures are more accurate.

The graphs are based on the Peng-Robinson equation of state (1) as improved by Stryjek and Vera (2, 3). The equations for thermodynamic properties using the Peng-Robinson equation of state are given in the appendix for volume, compressibility factor, fugacity coefficient, residual enthalpy, and residual entropy. Critical constants and ideal gas heat capacities for use in the equations are from the data compilations of DIPPR (8) and Yaws (28, 29, 30).

The literature has been carefully searched in construction of the graphs. References for sources used in preparing the work are given in the section following the graphs near the end of the book.

For the graphs, some of the compounds may undergo thermal decomposition (reaction) at the higher temperatures. For such cases of thermal decomposition, the graphs are useful for ascertaining property values of the pure compound which is contained in the reaction mixture. Chemistry handbooks and DIPPR (8) notes may be used for specifics regarding thermal decomposition.

A list of compounds is given near the end of the book to aid the user in quickly locating compounds of interest from knowledge of the chemical formula or name.

An executable computer program, complete with data files, is available for calculation of thermodynamic properties. For information on the program, contact Carl L. Yaws, Ph.D., P. O. Box 10053, Beaumont, Texas 77710, phone/fax (409) 880-8787.

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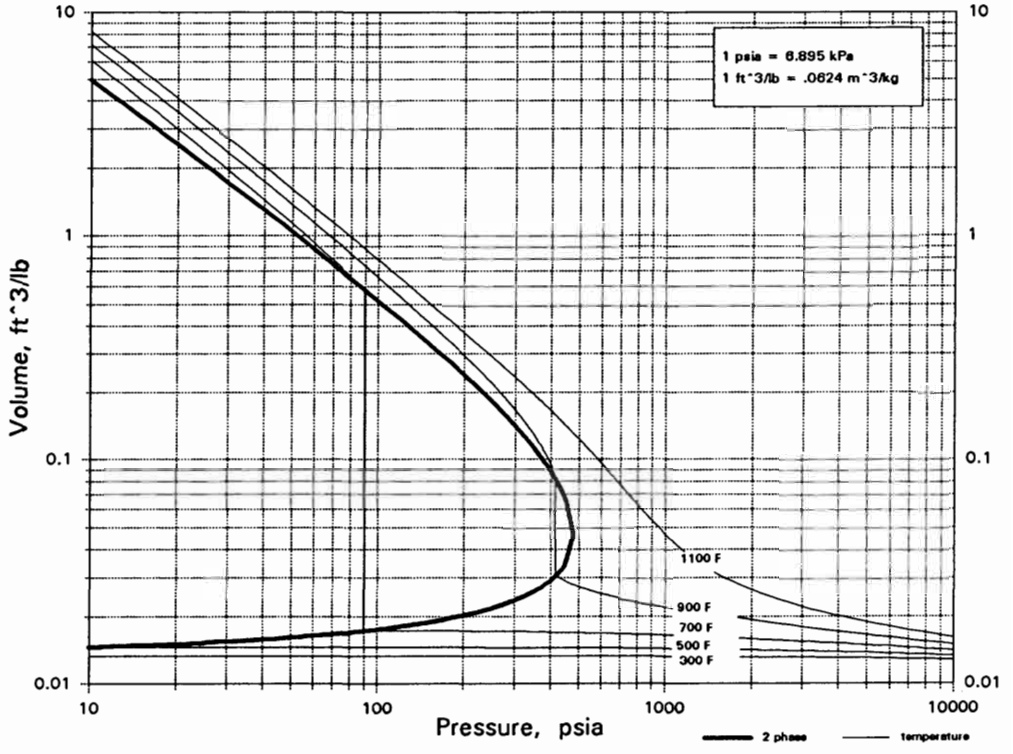
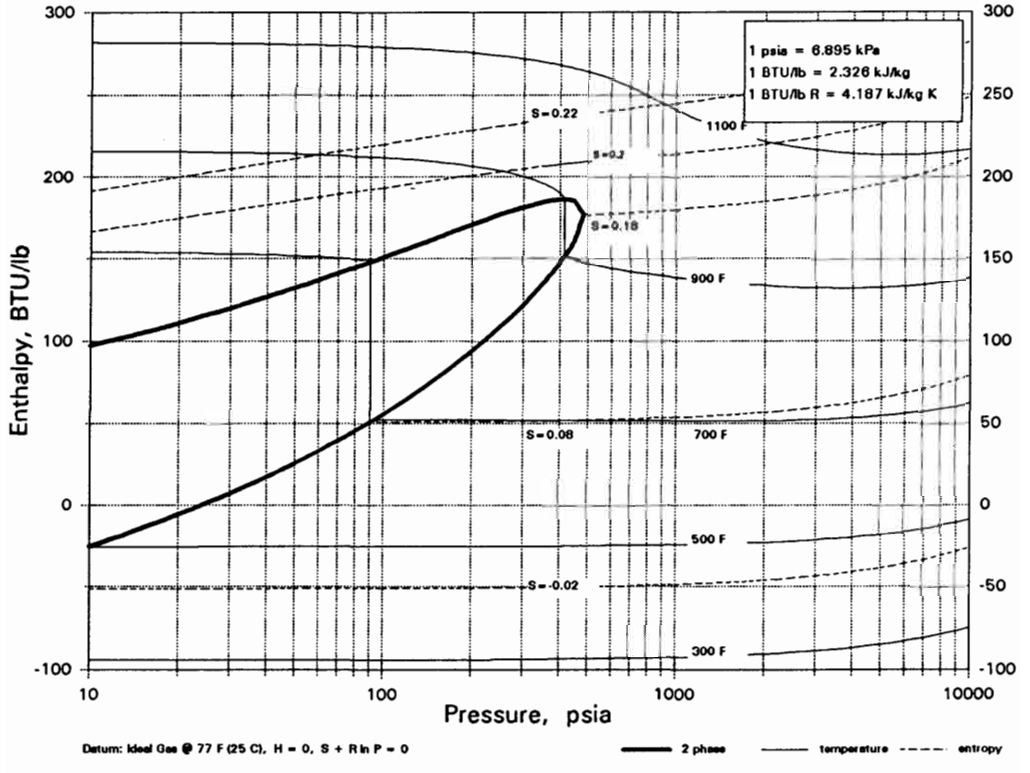
C8H4Cl2O2 ISOPHTHALOYL CHLORIDE





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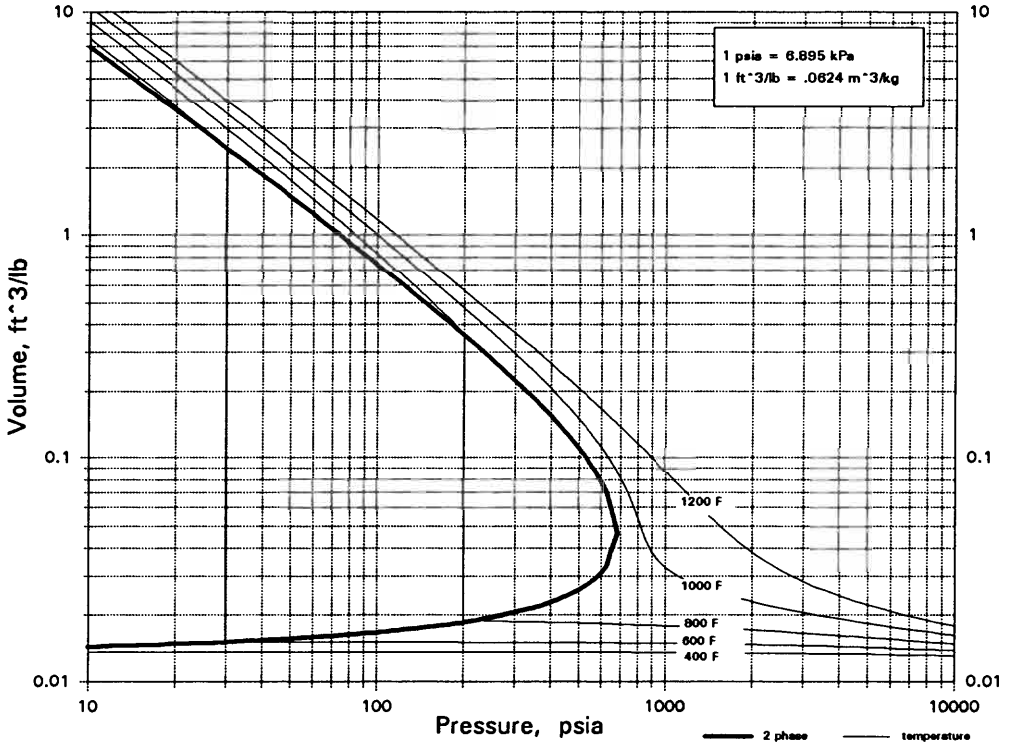

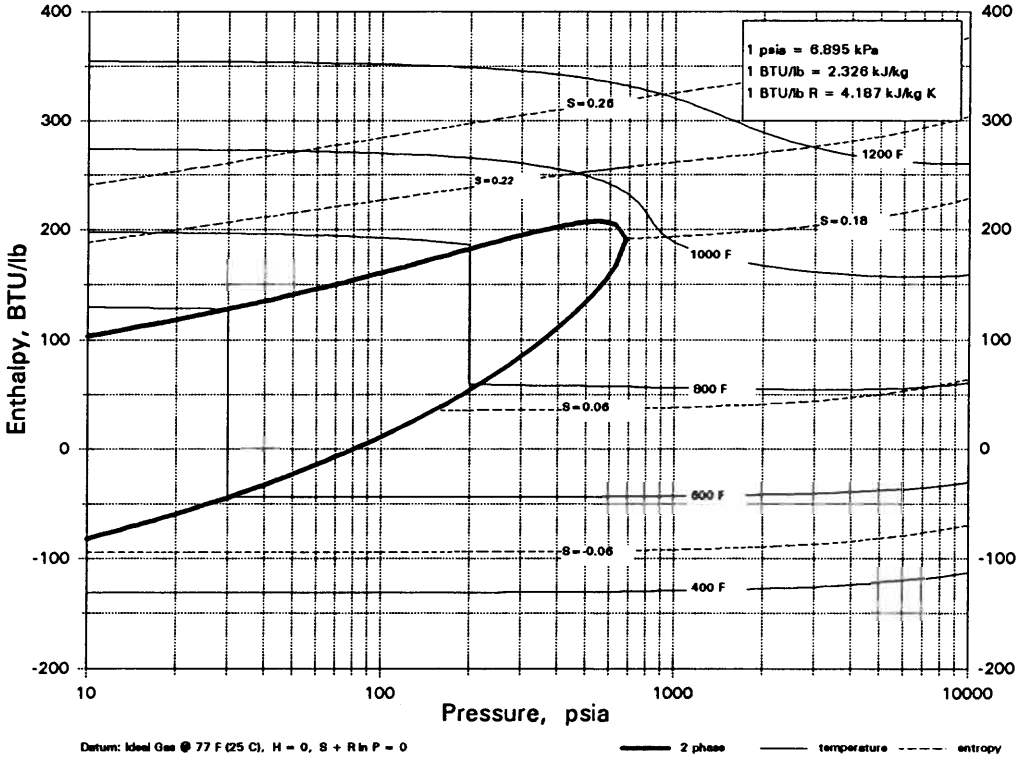

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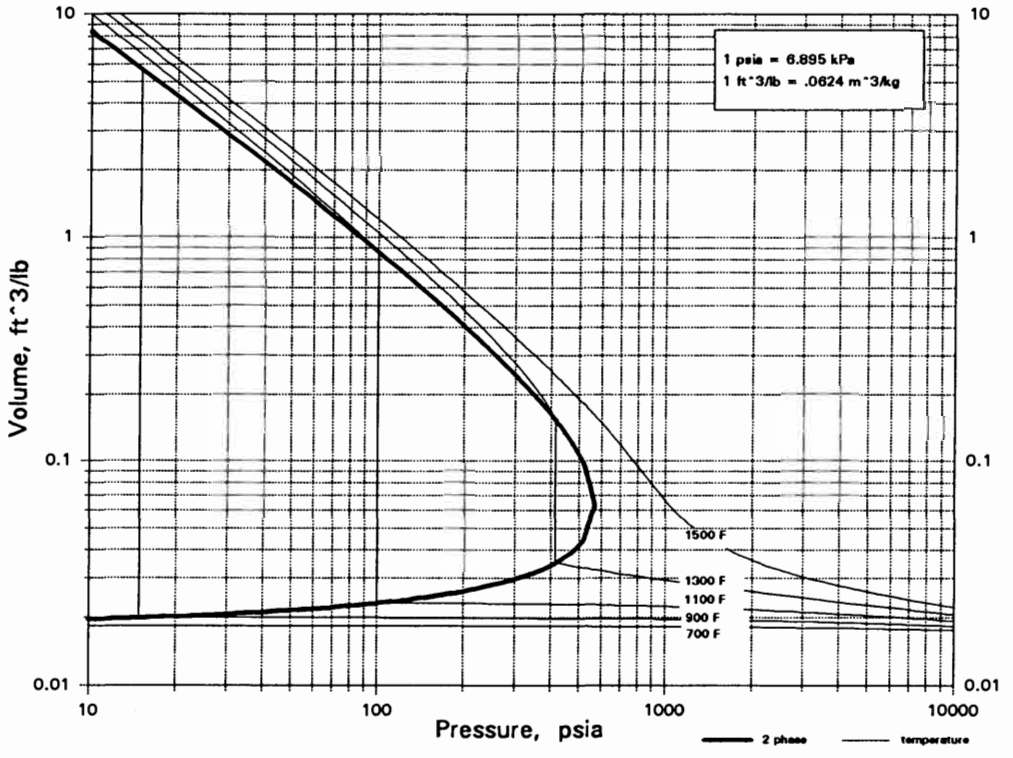

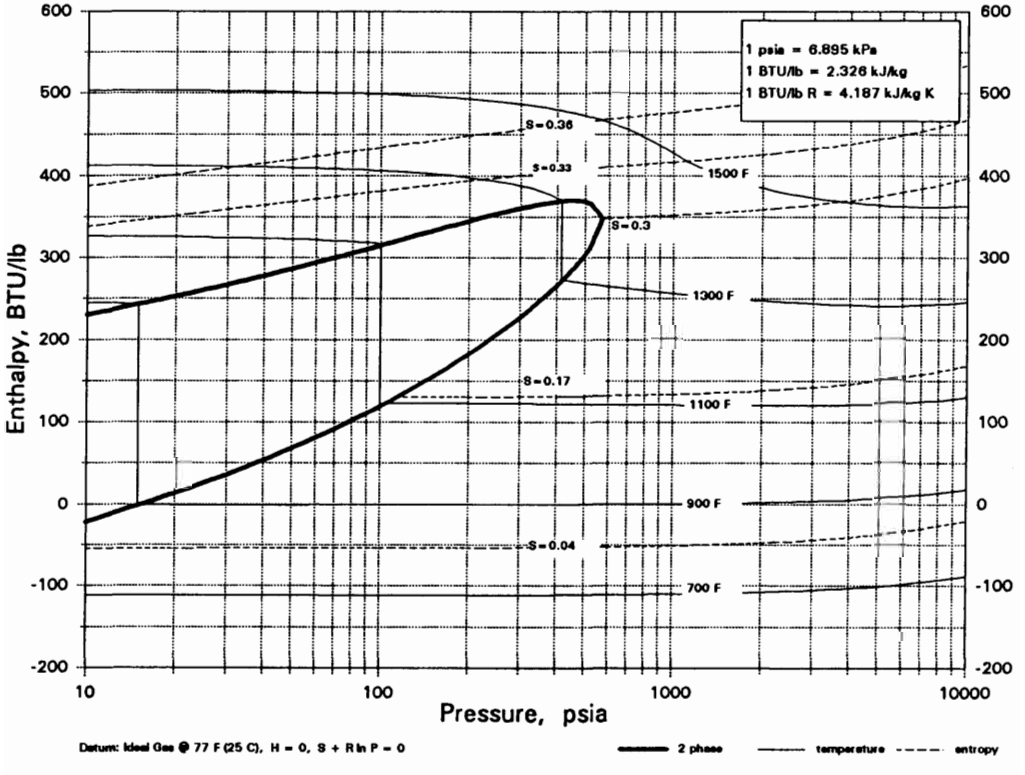

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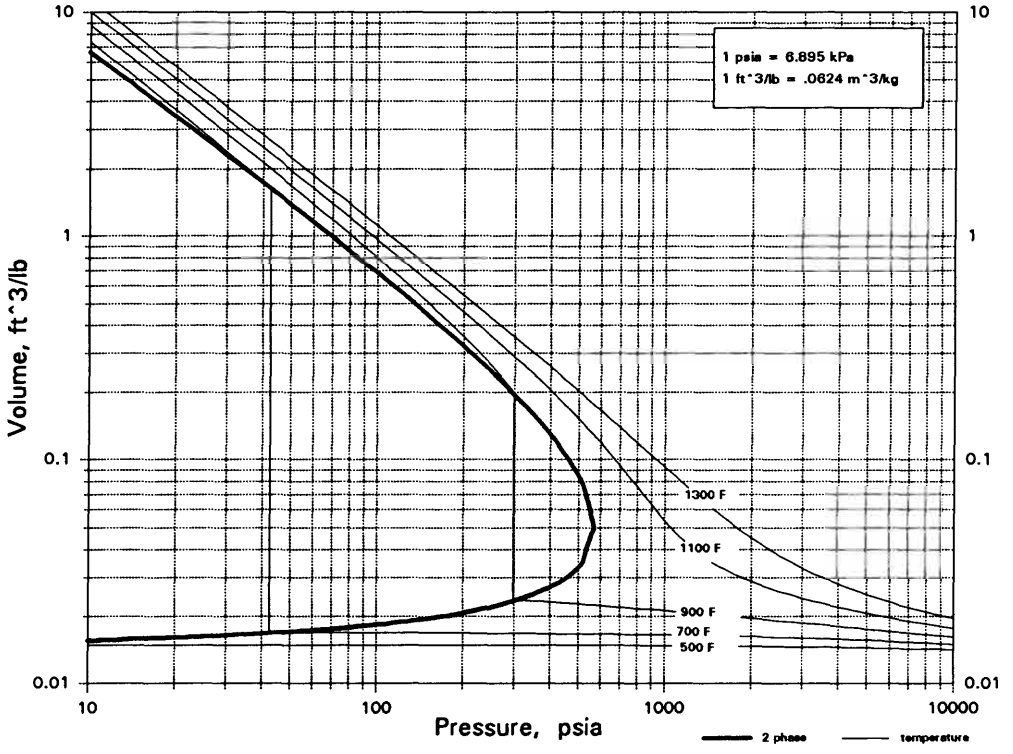

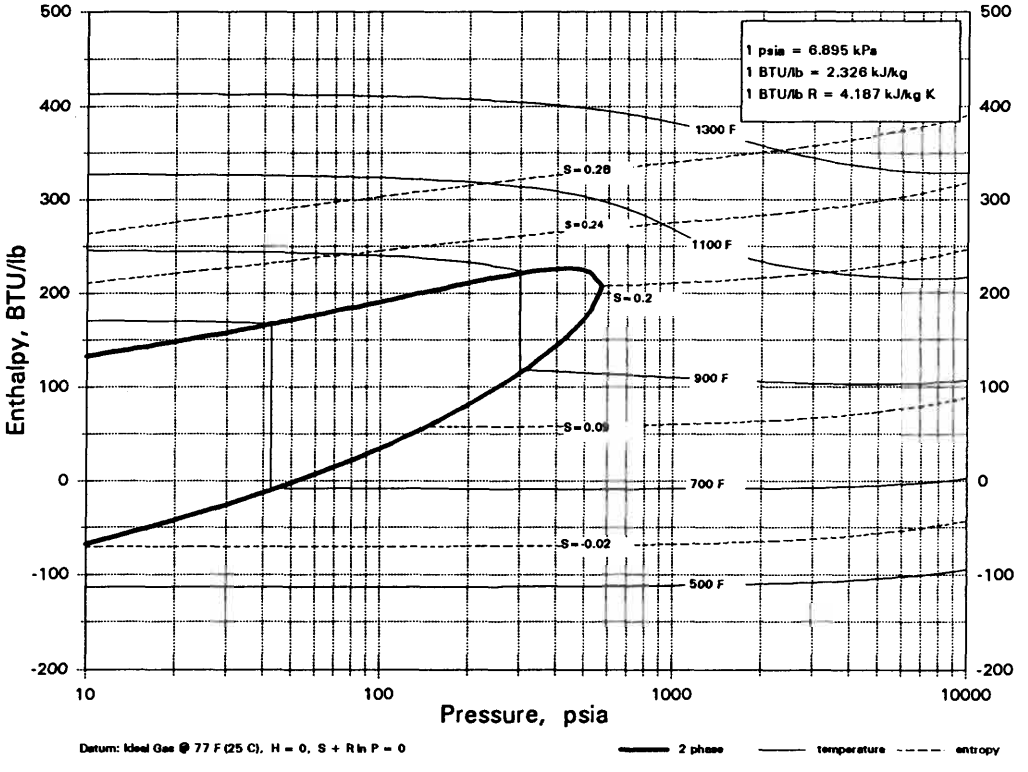

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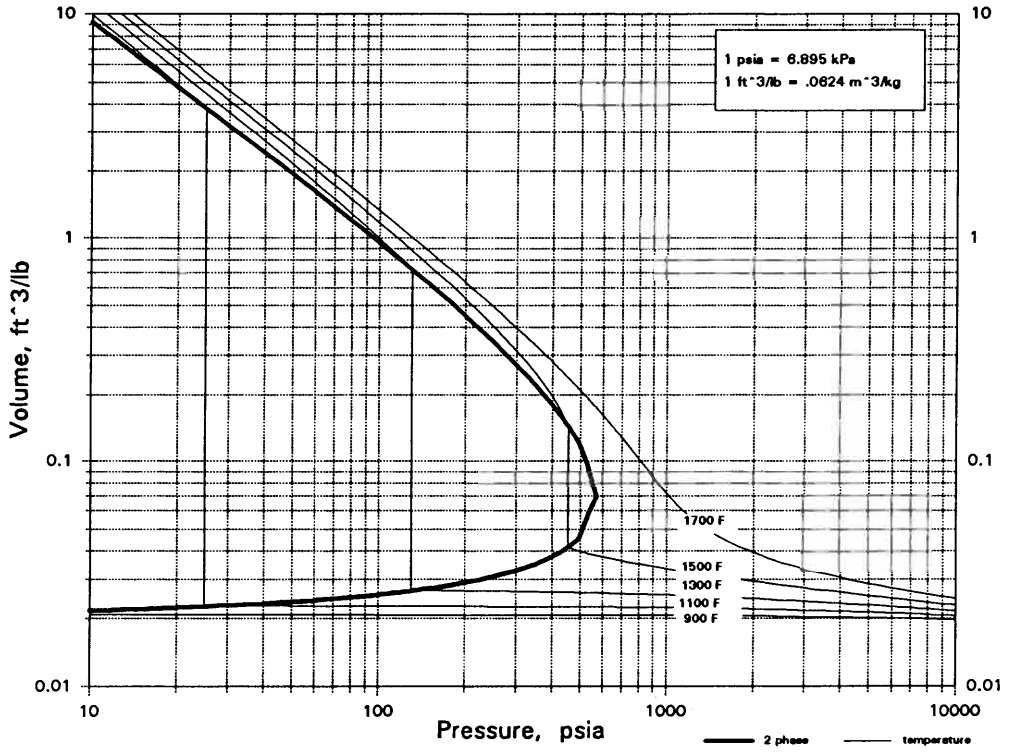

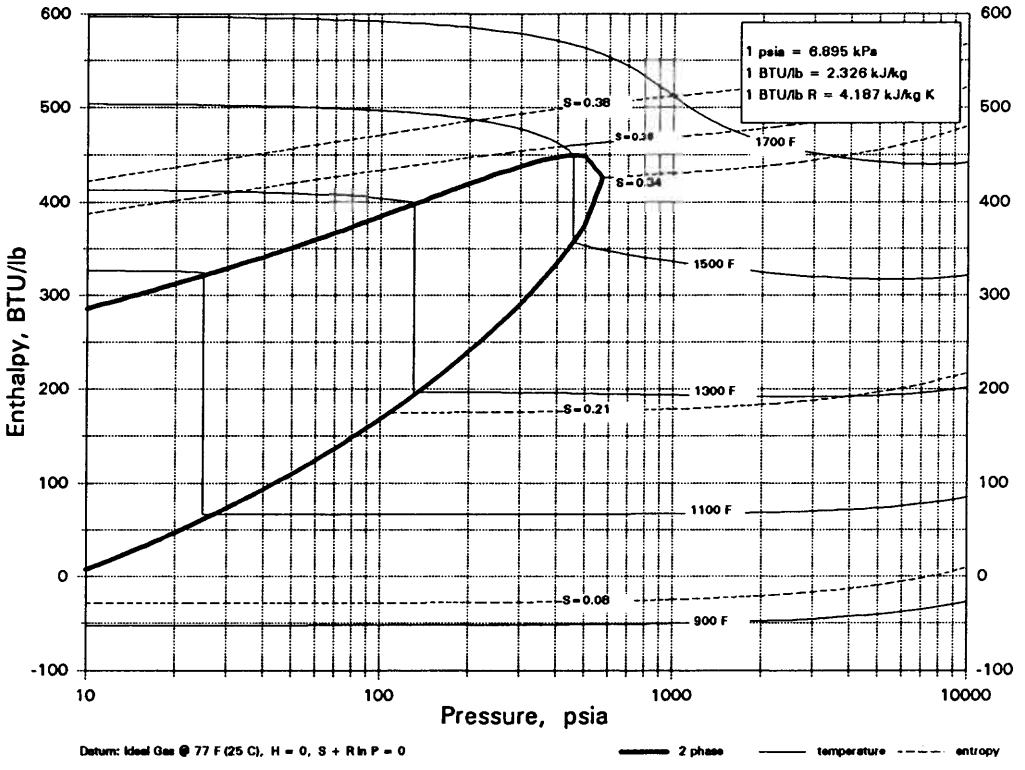

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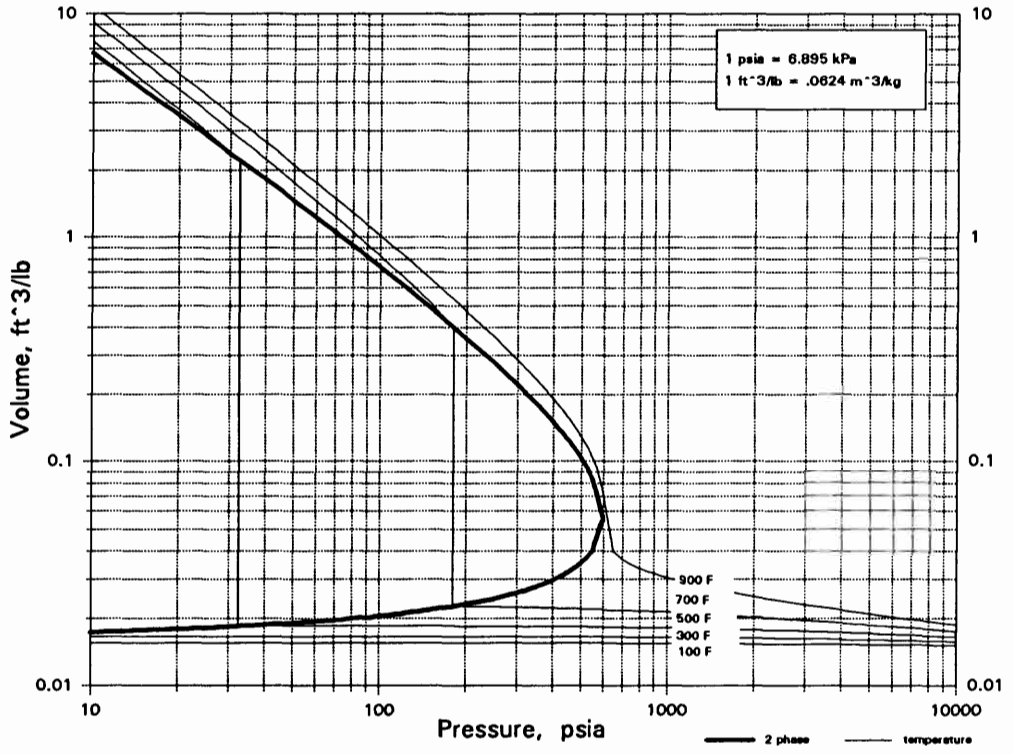

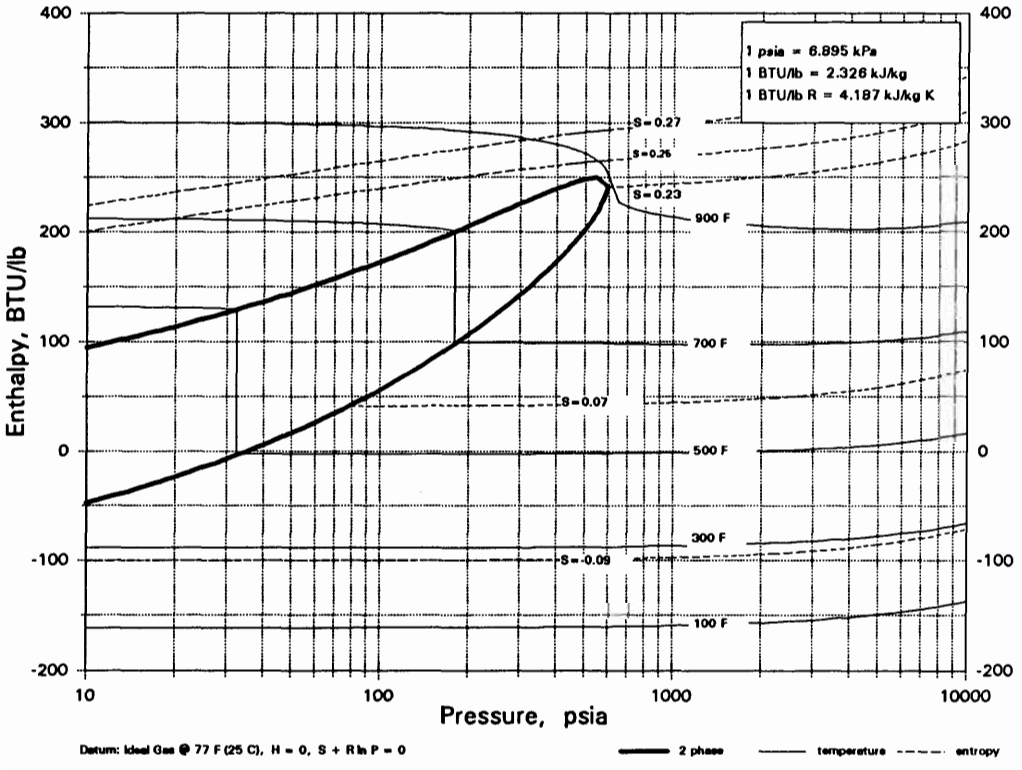

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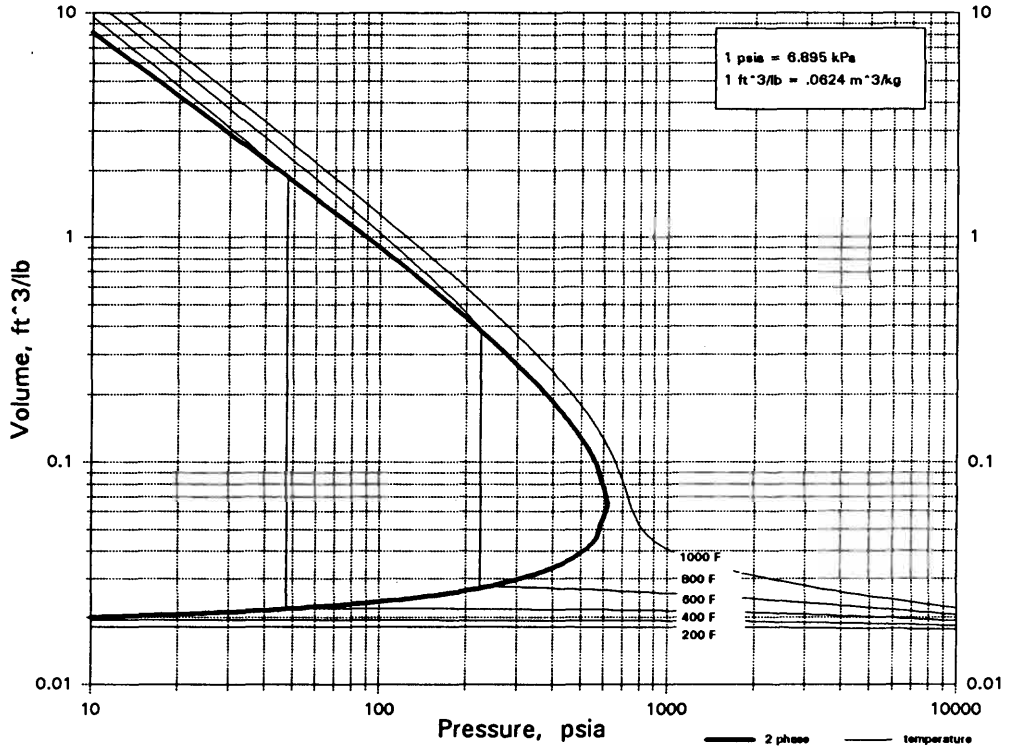

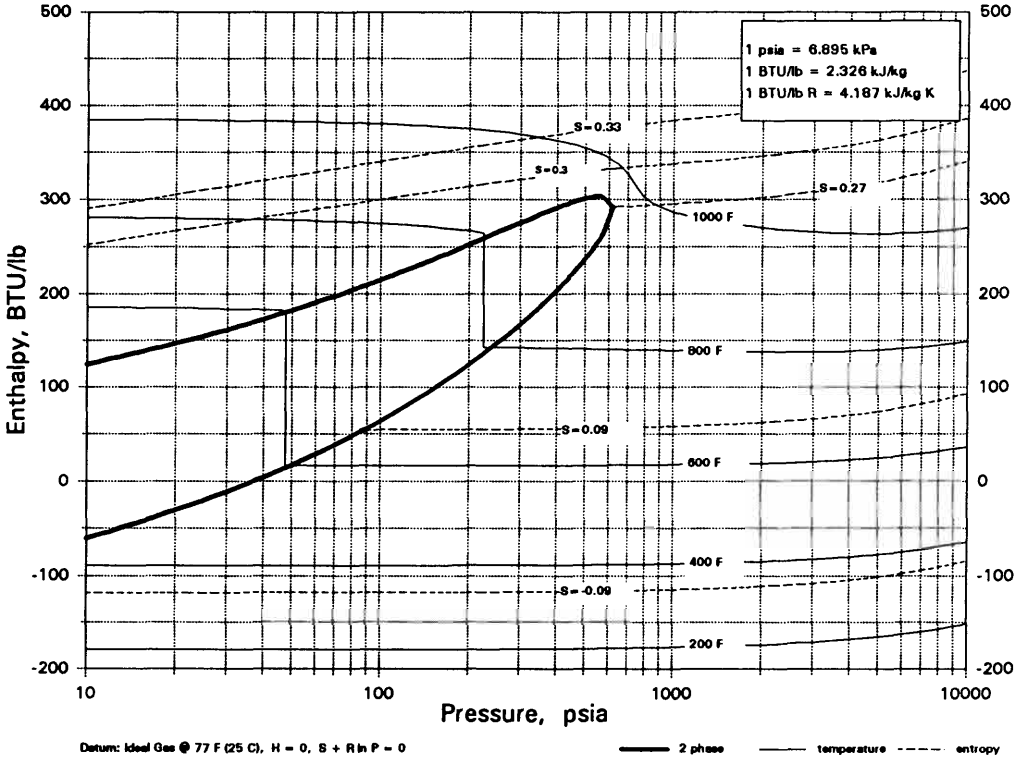

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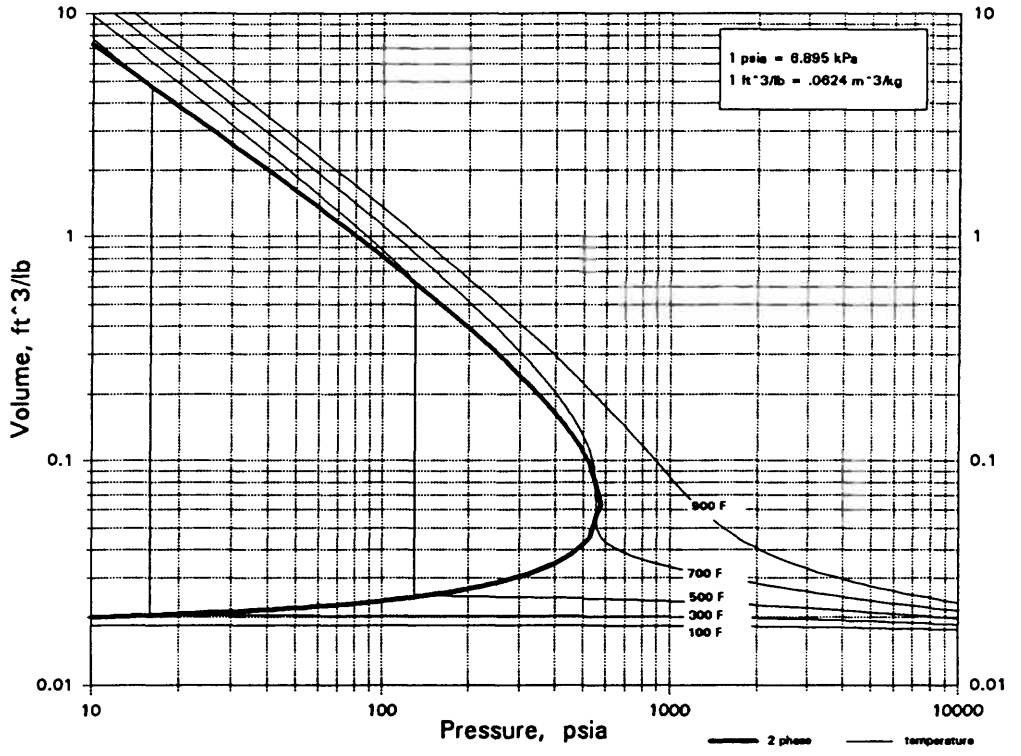

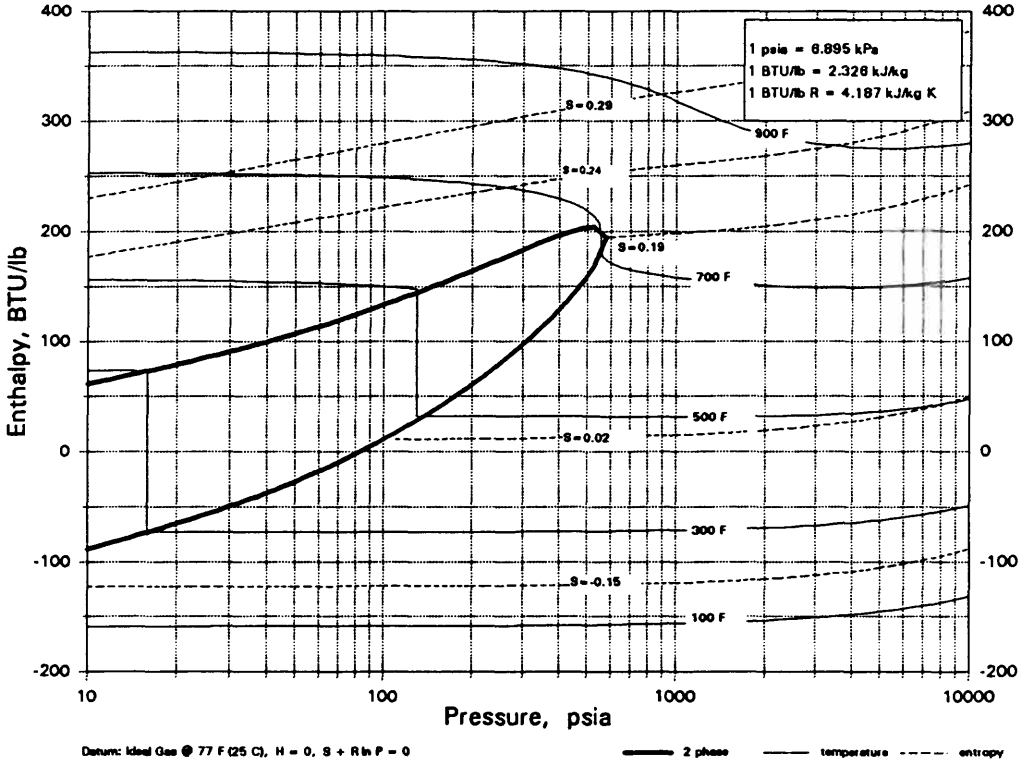

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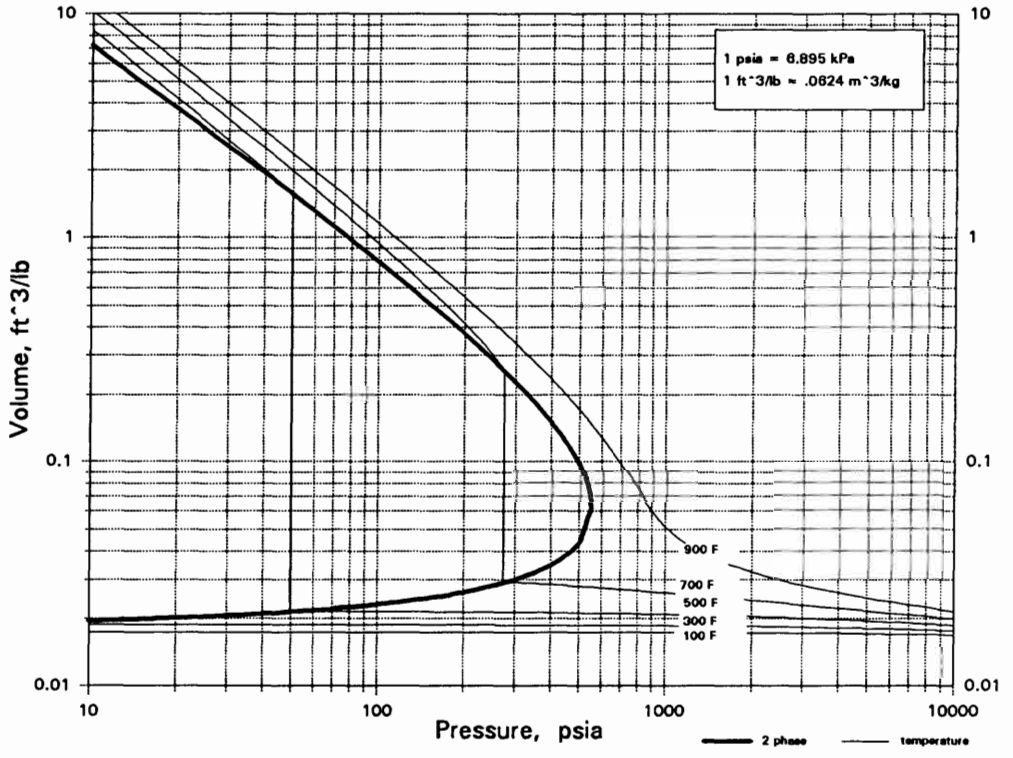

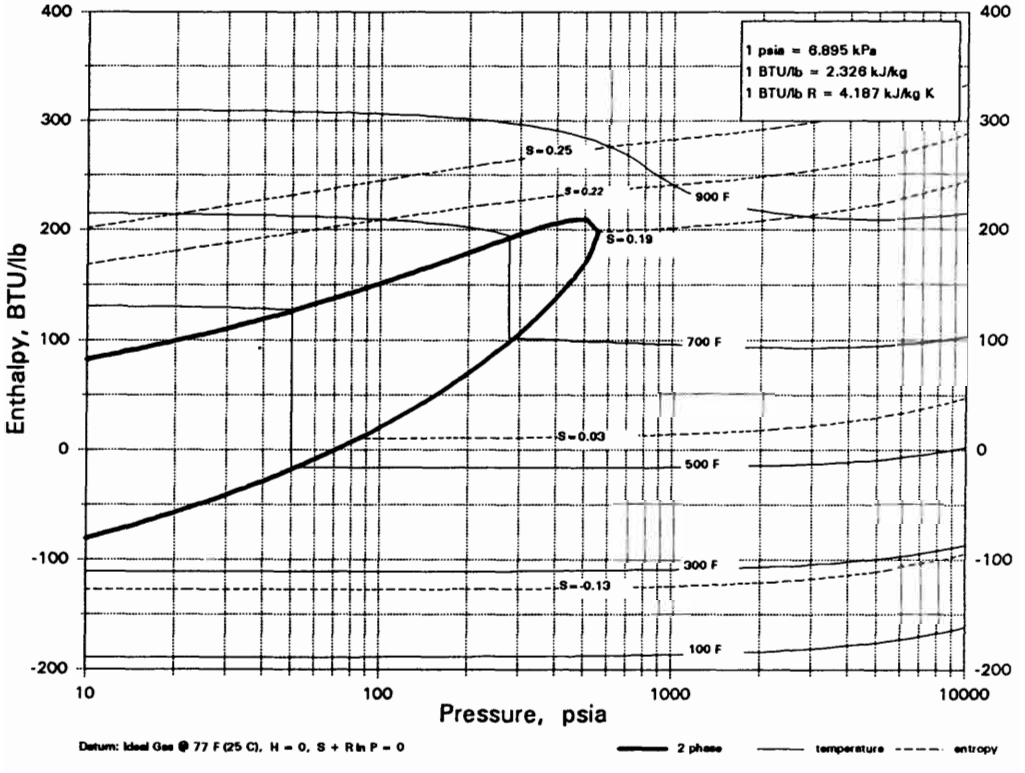

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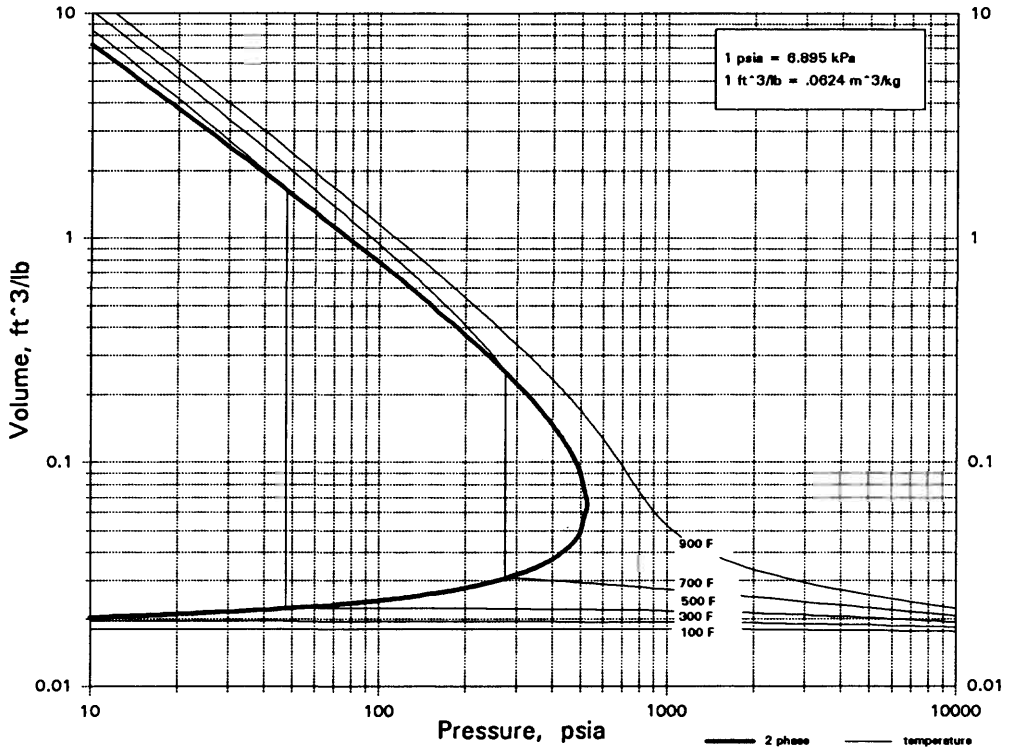

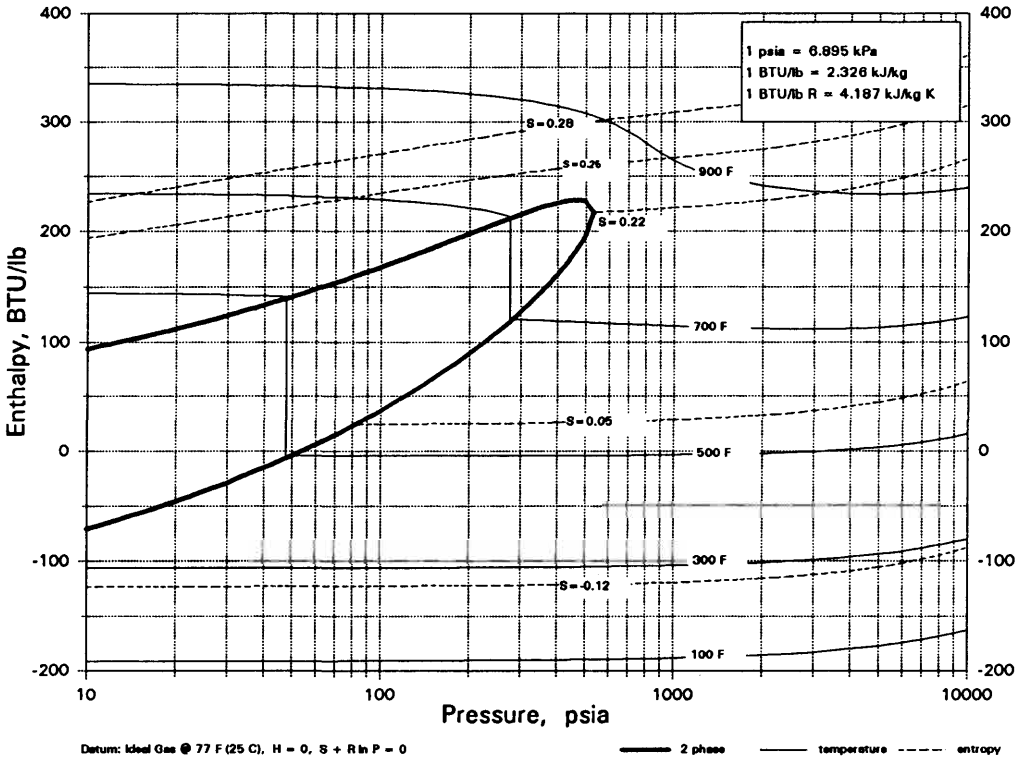

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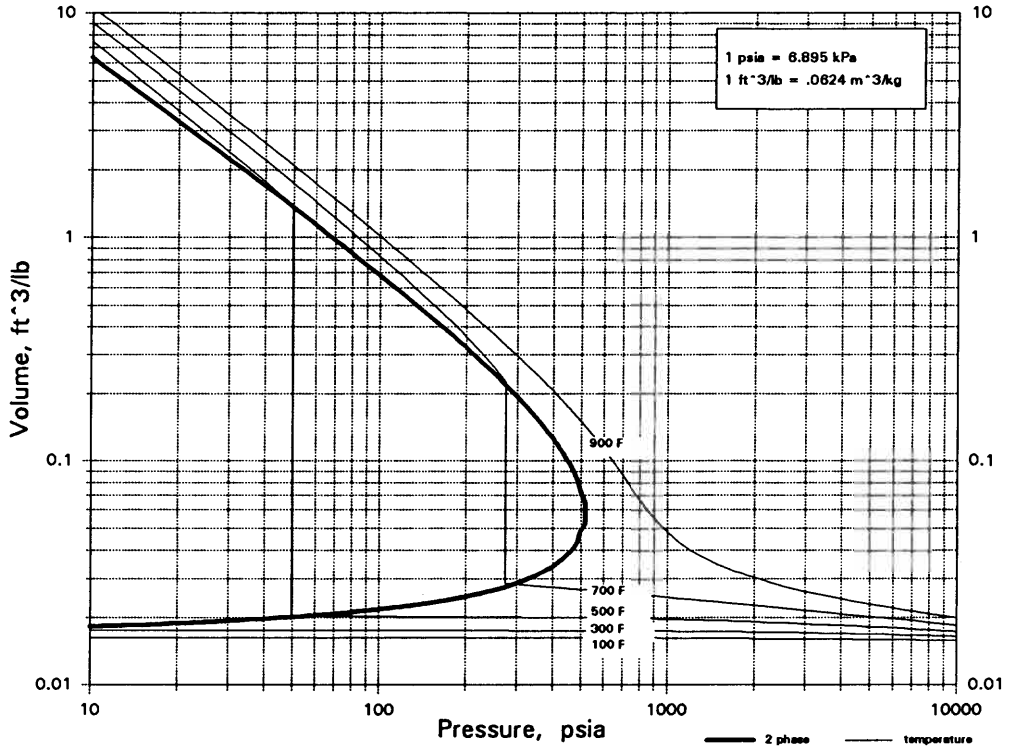

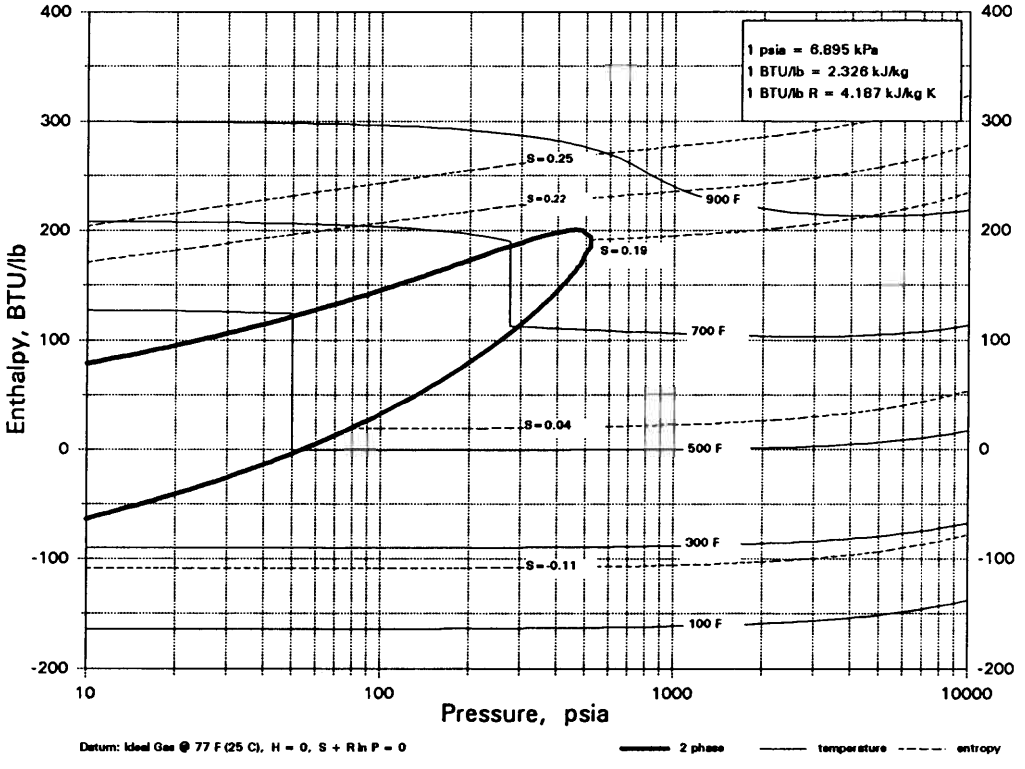

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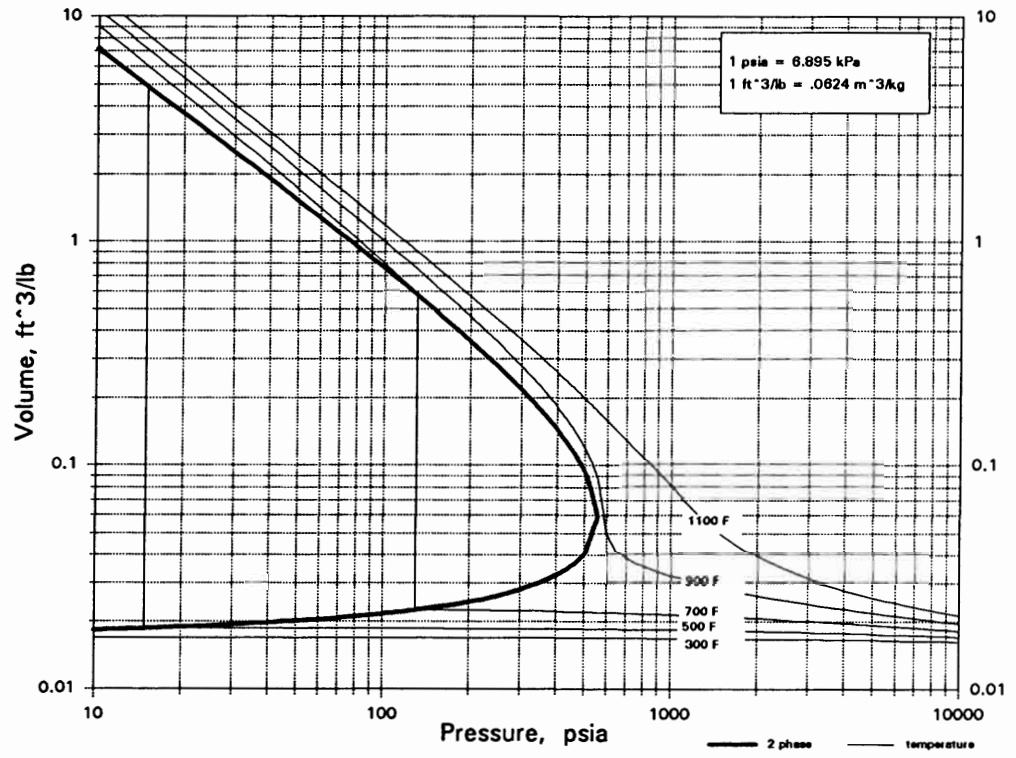

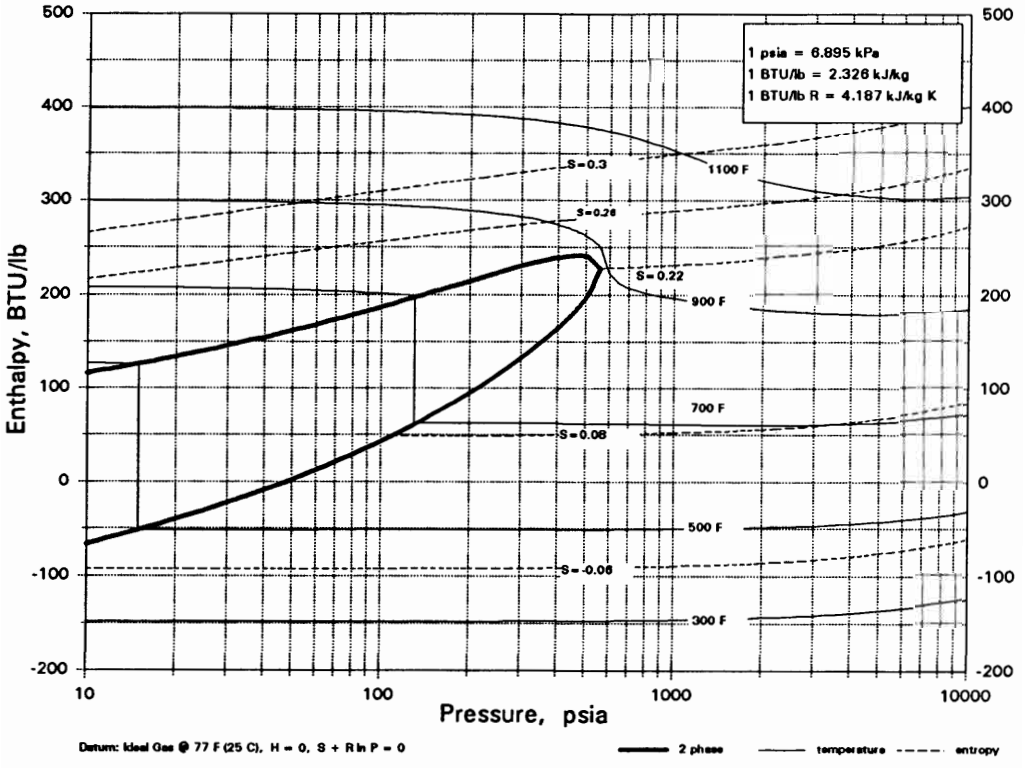

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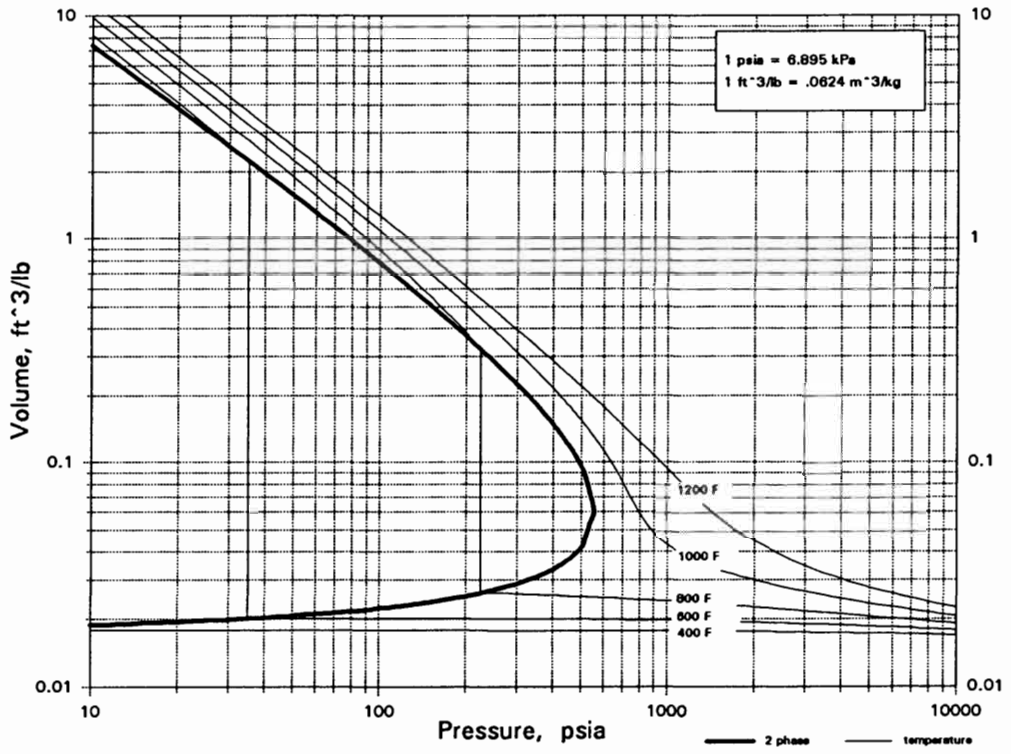

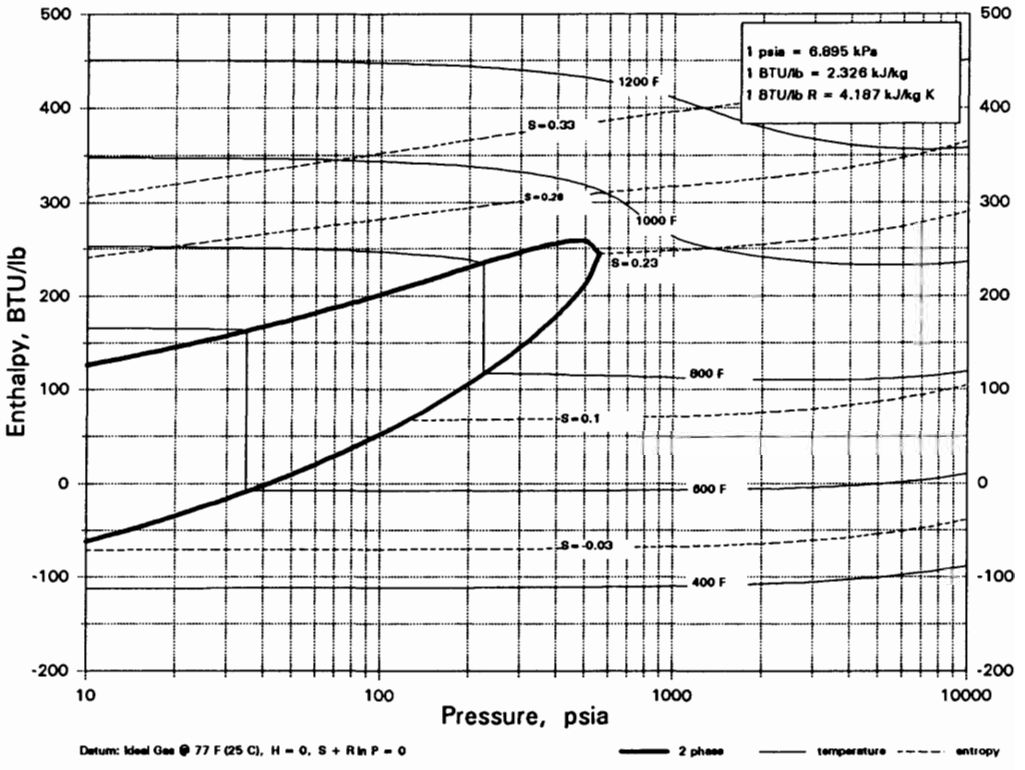

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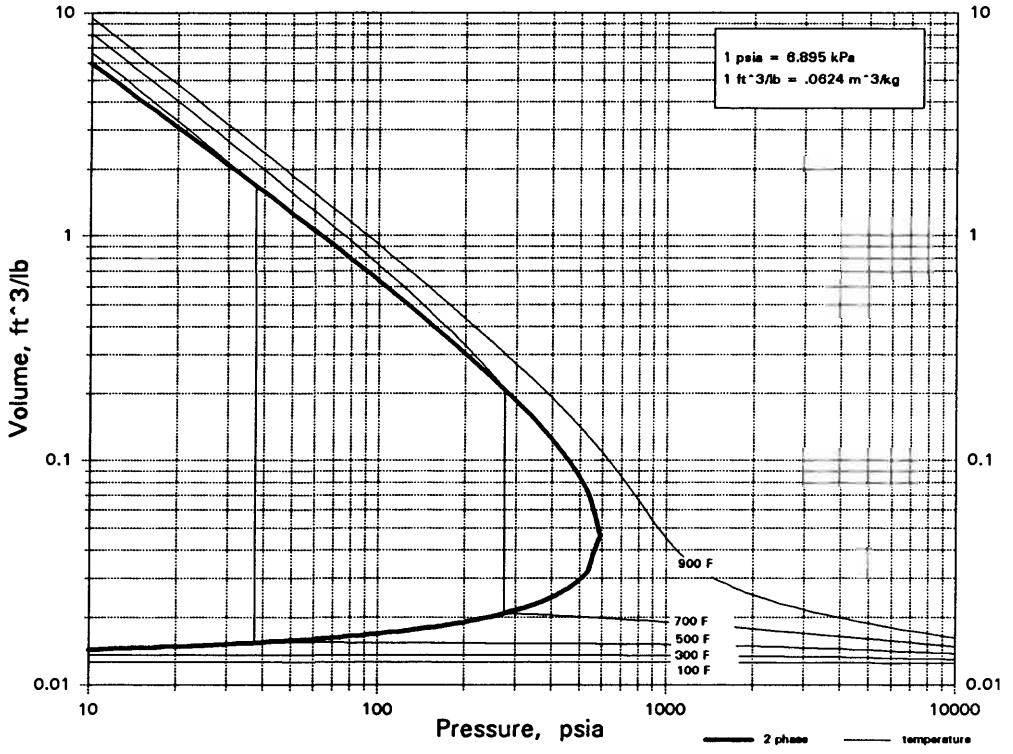

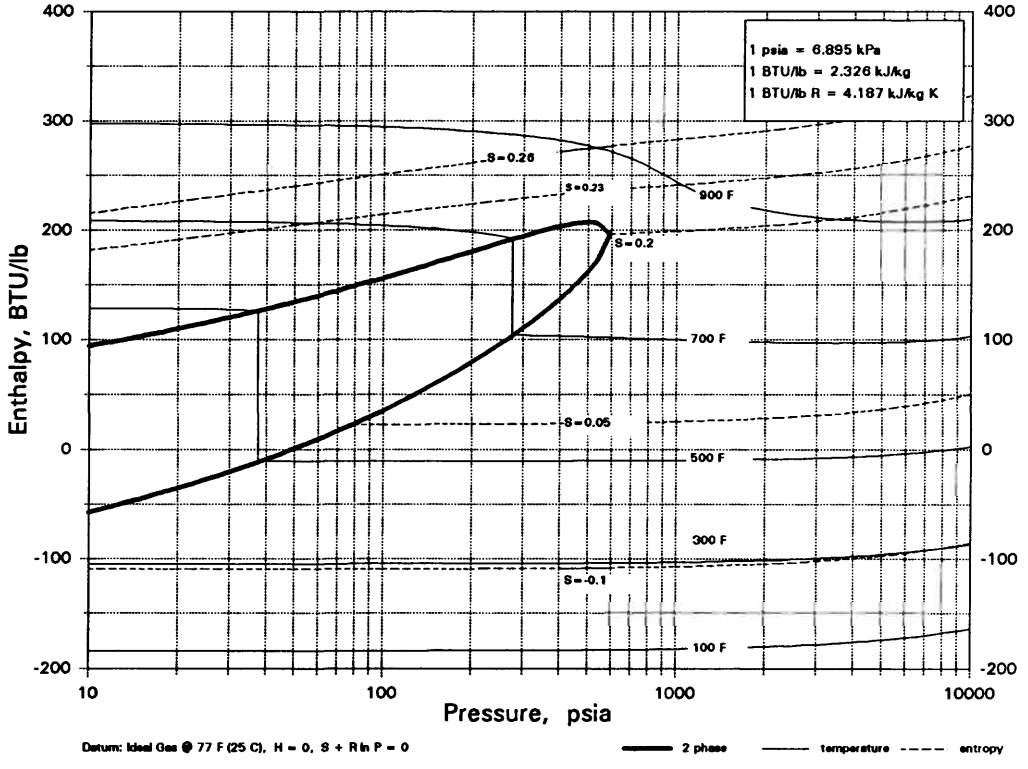

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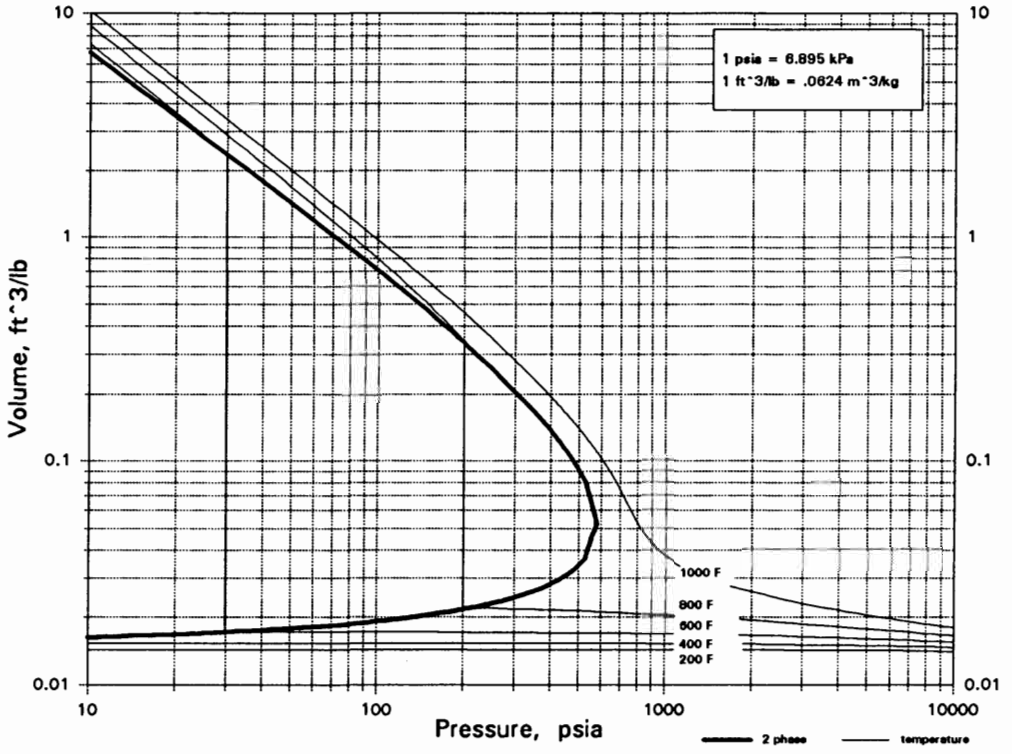

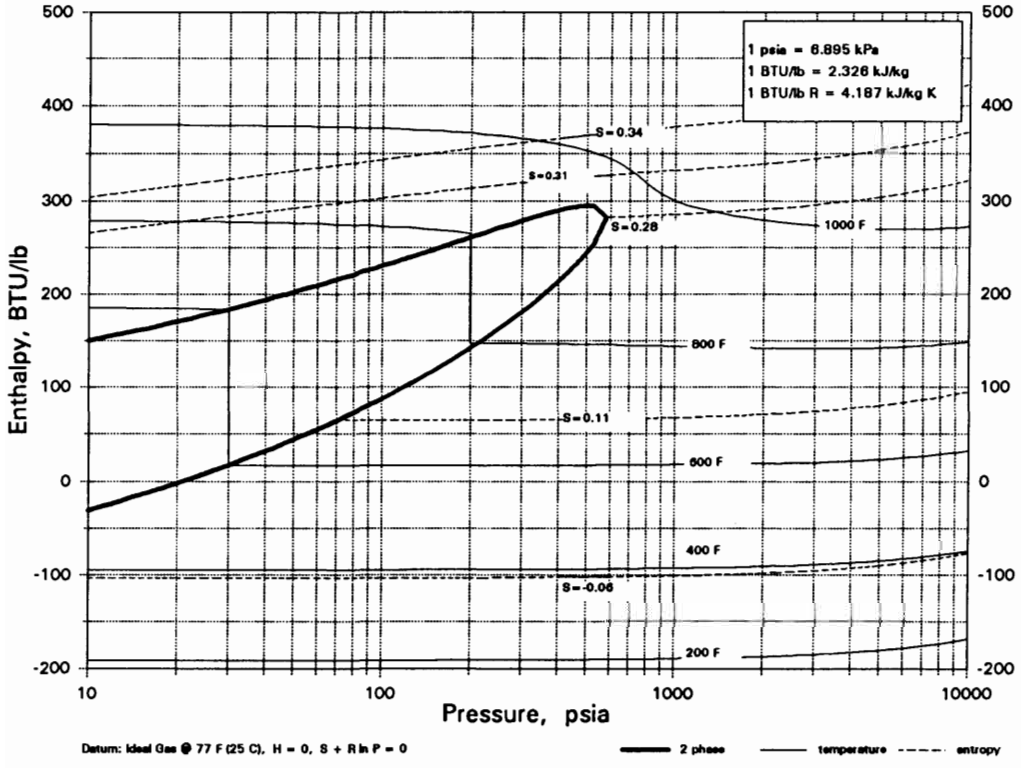

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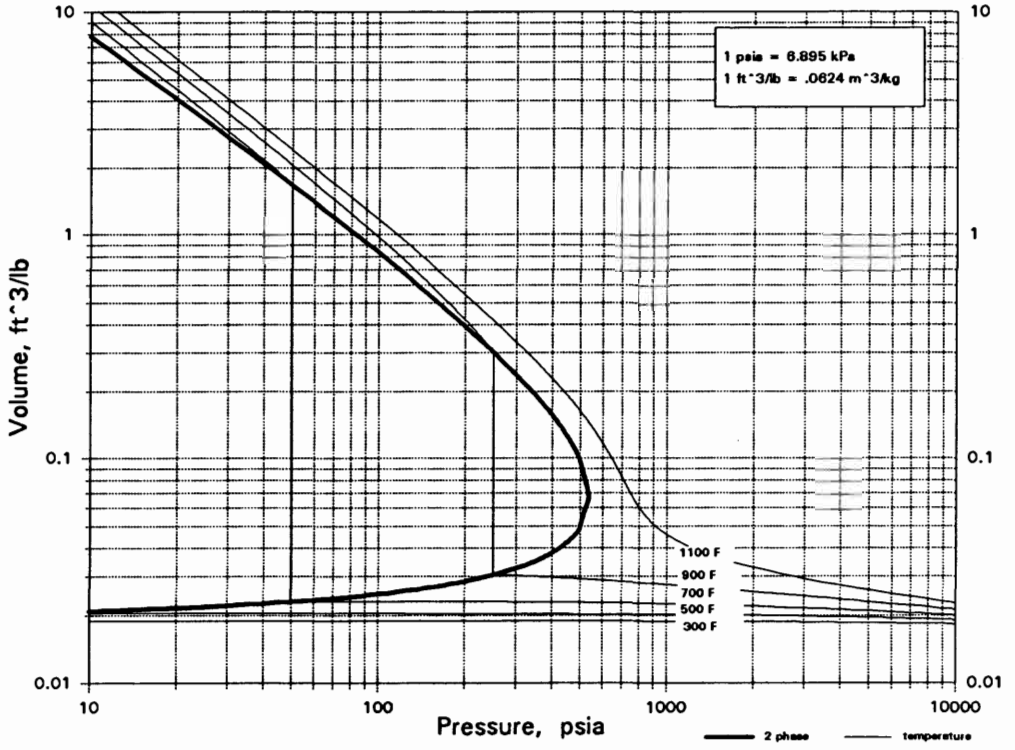

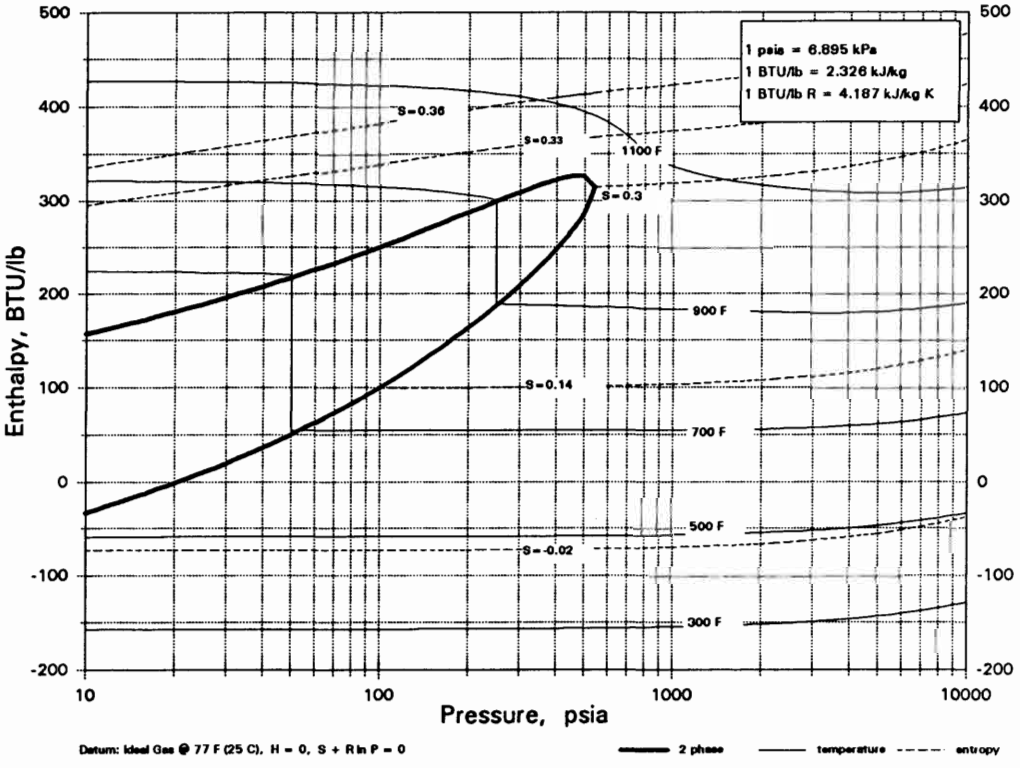

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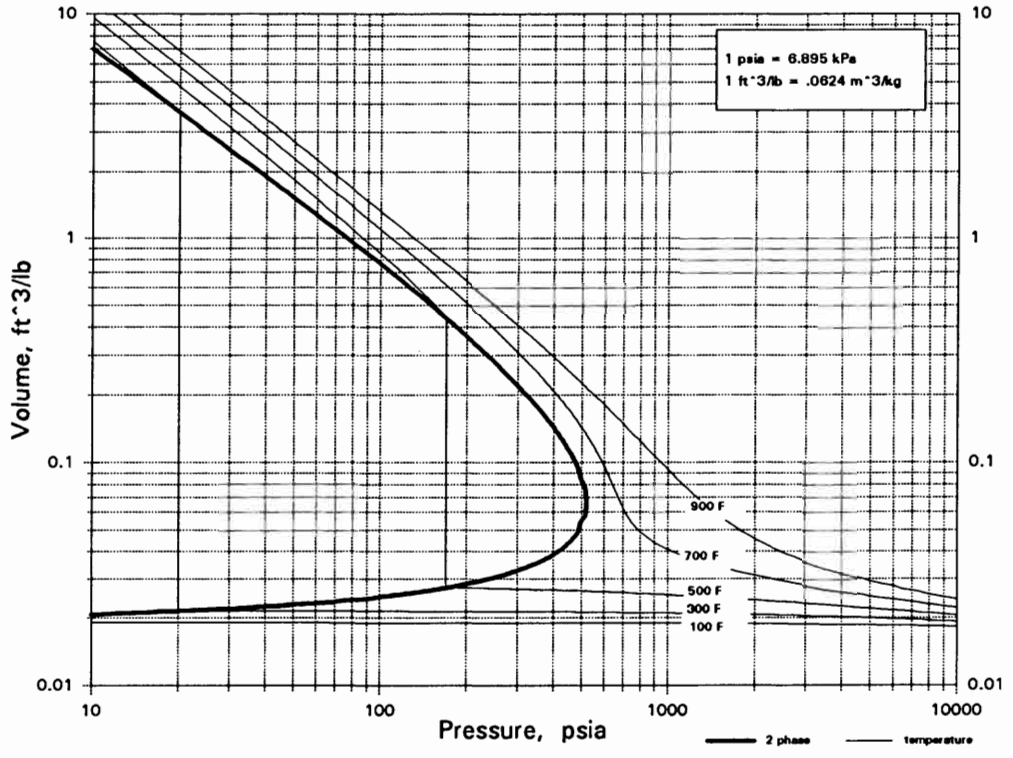

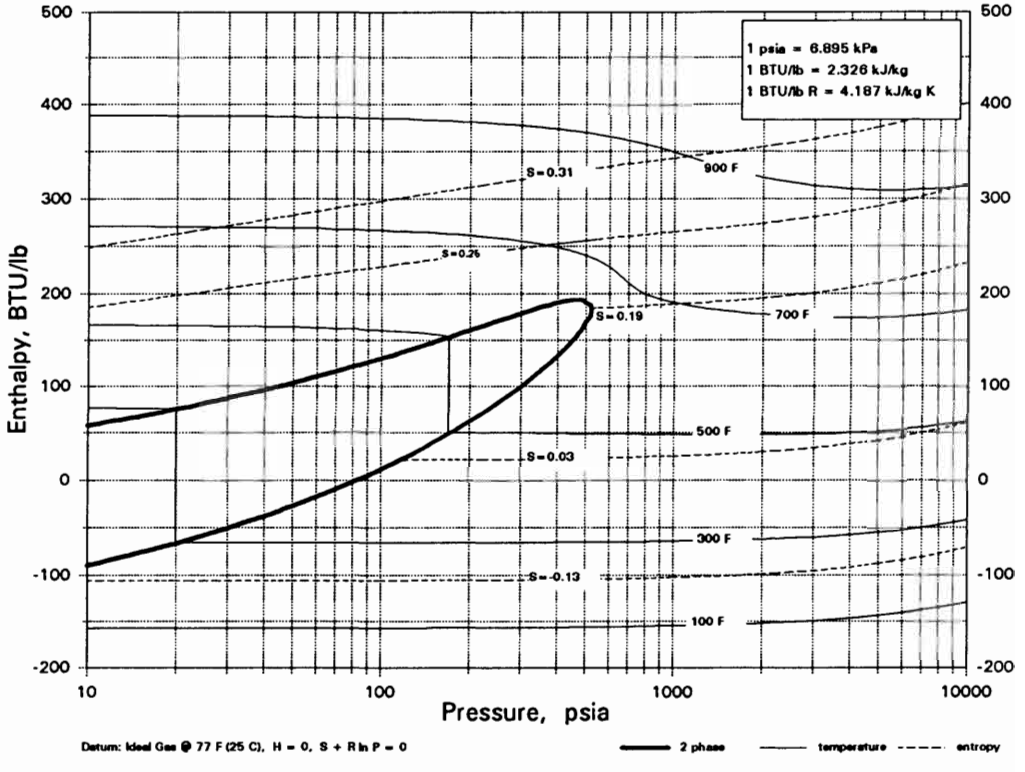

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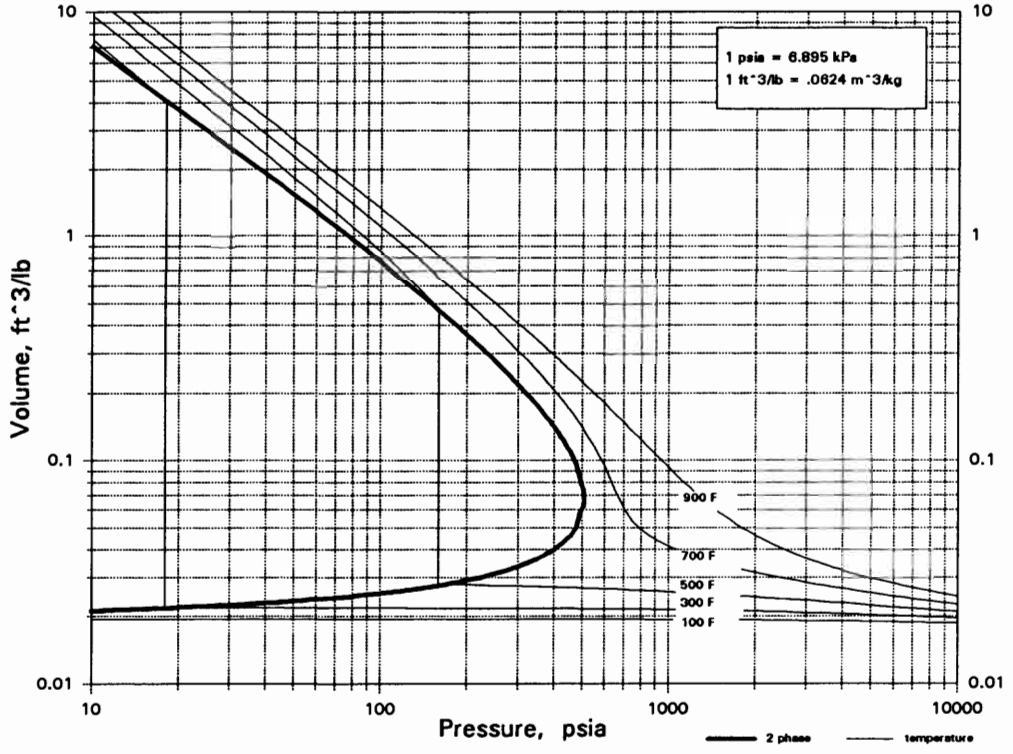

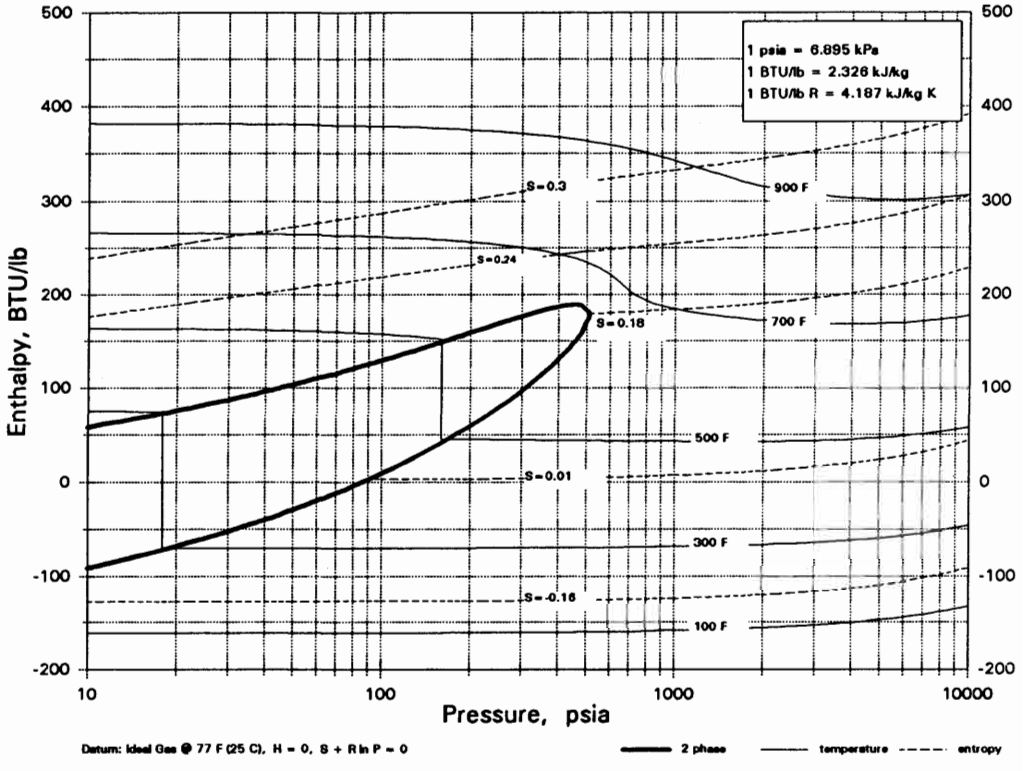

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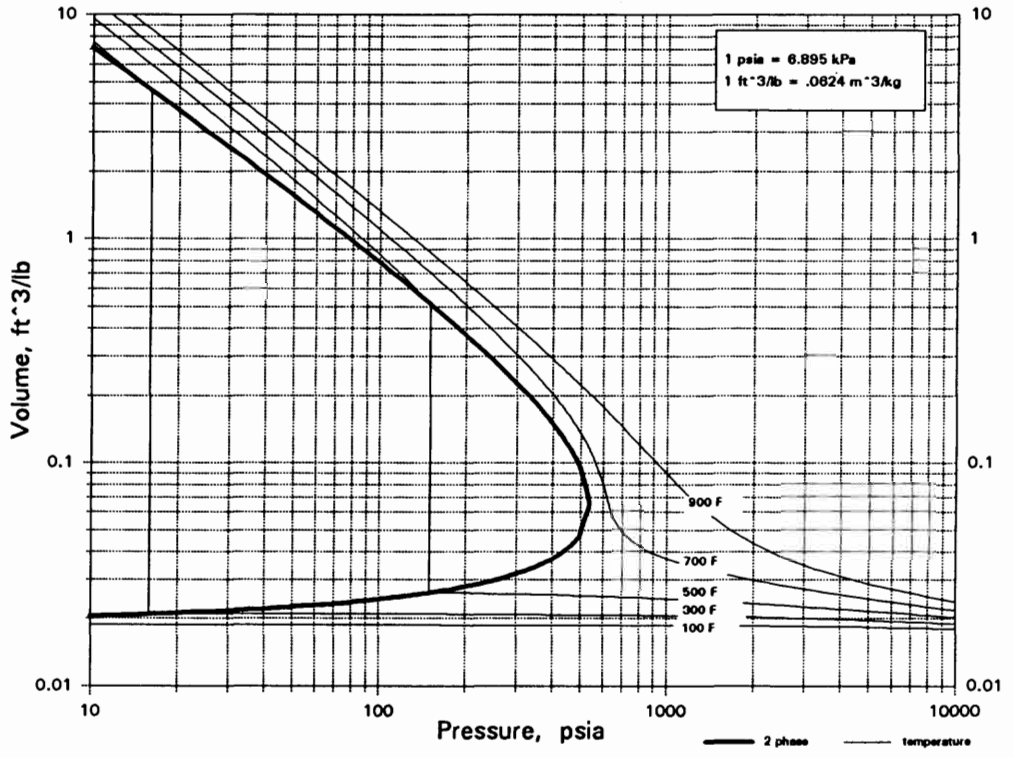

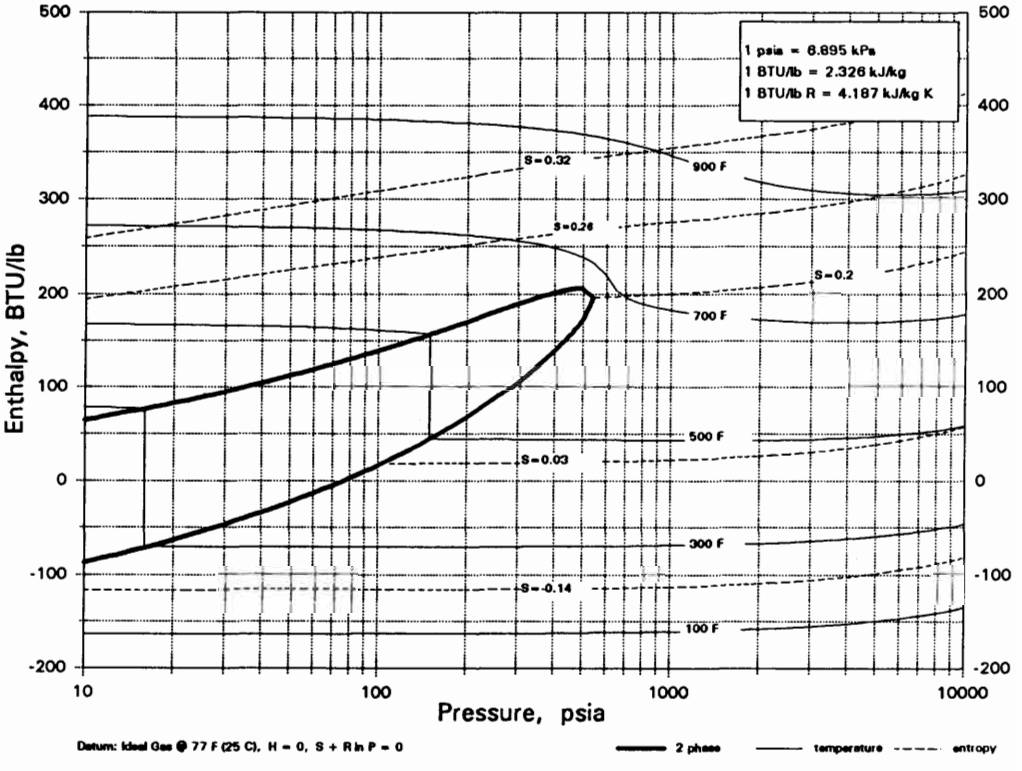

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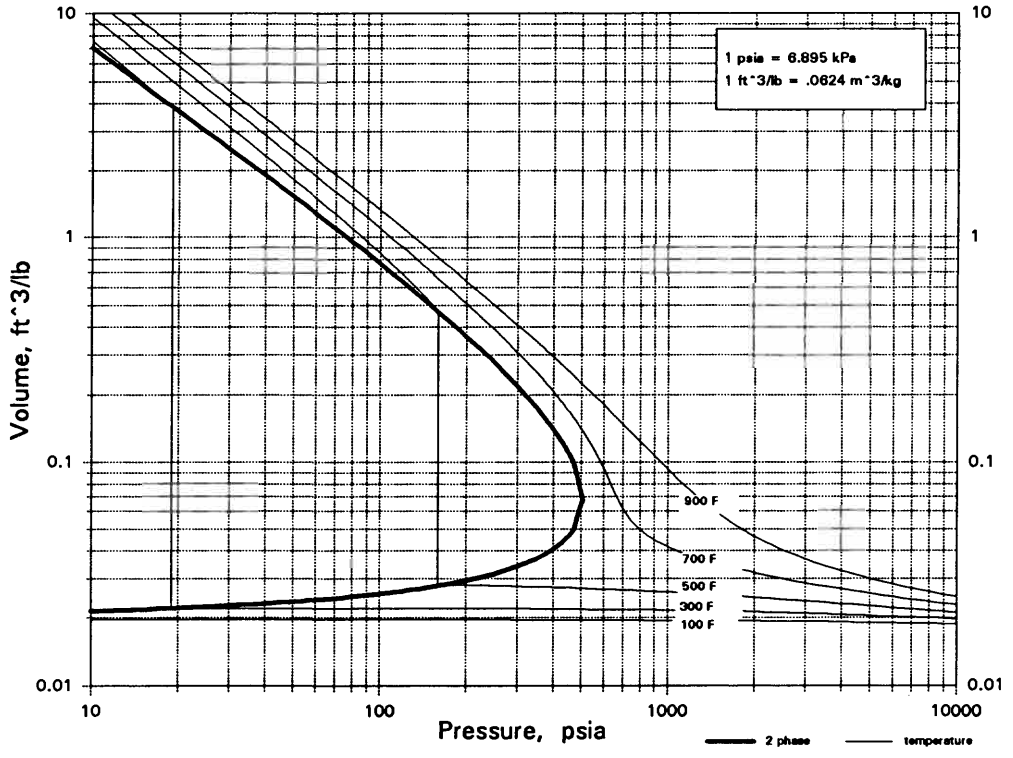

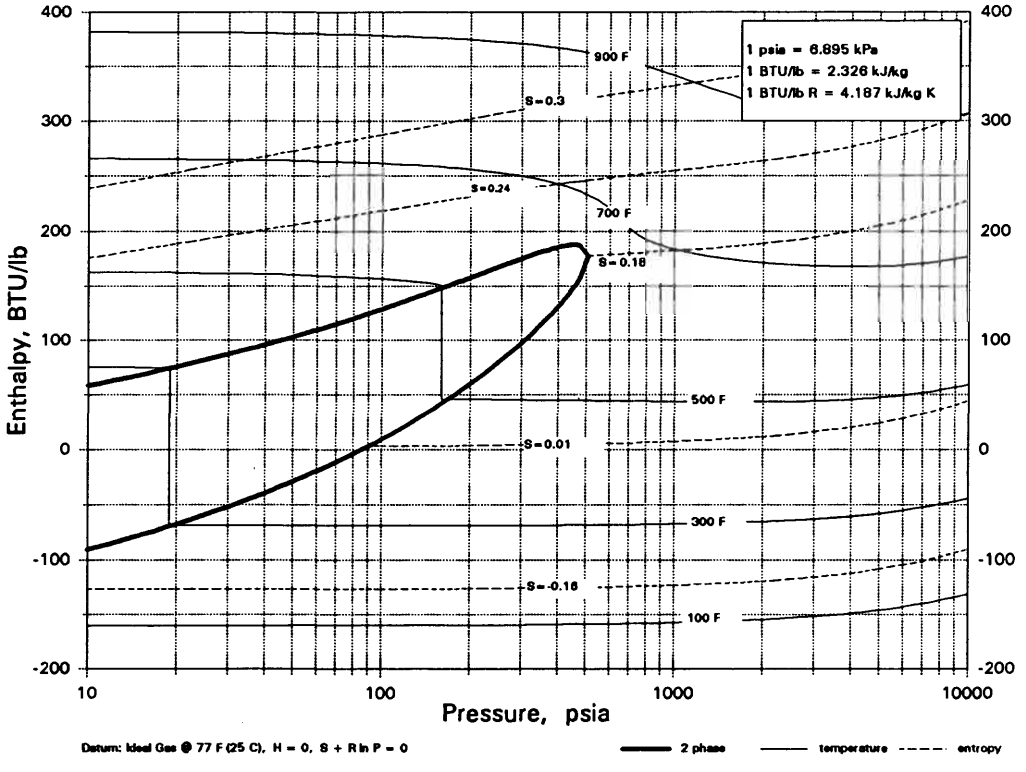

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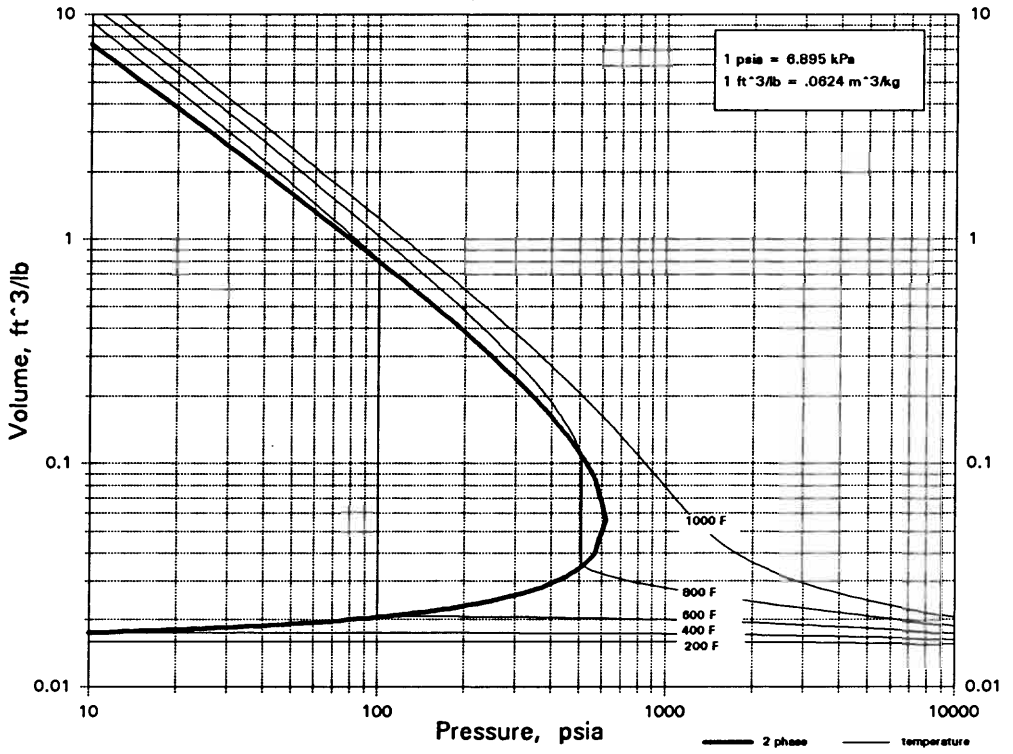

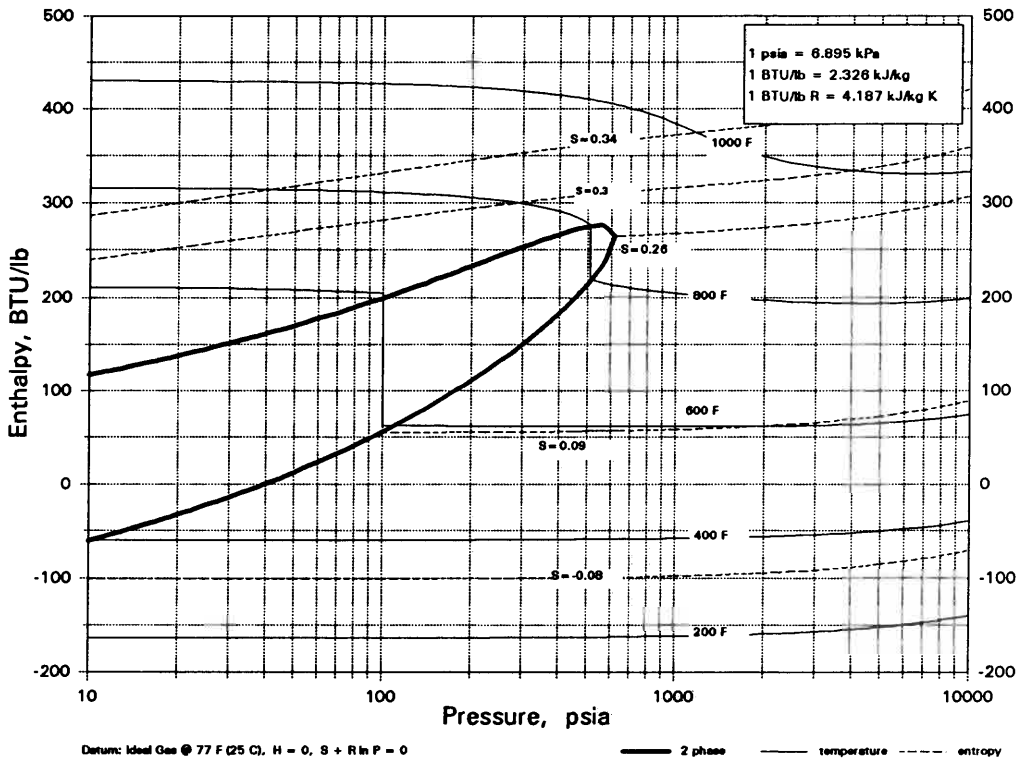

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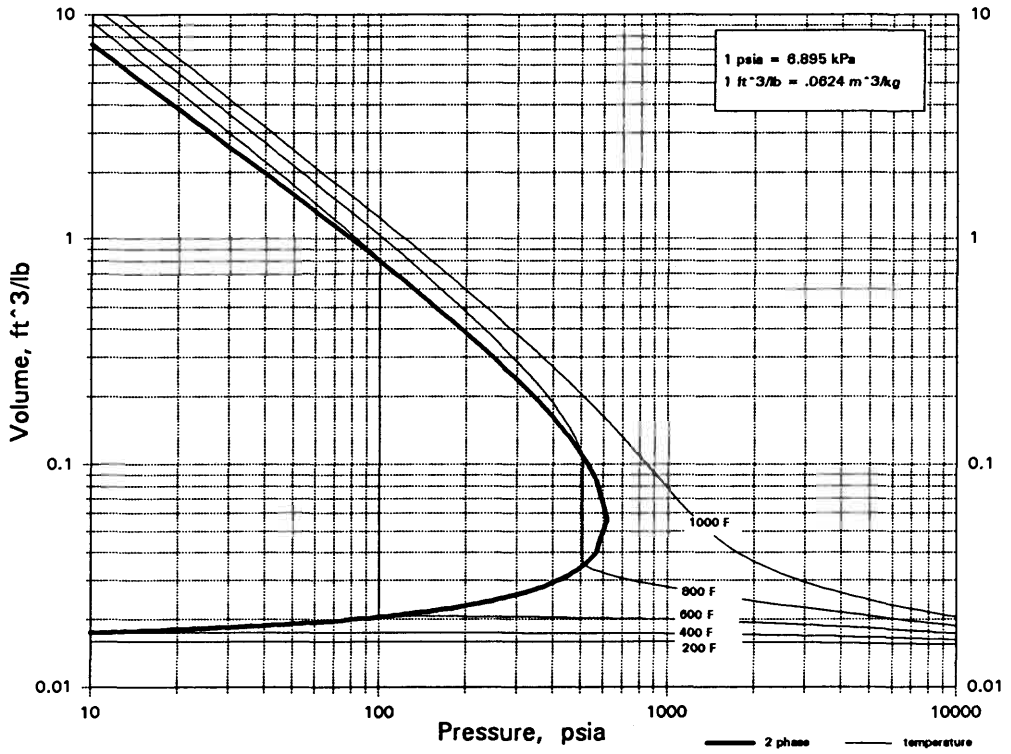
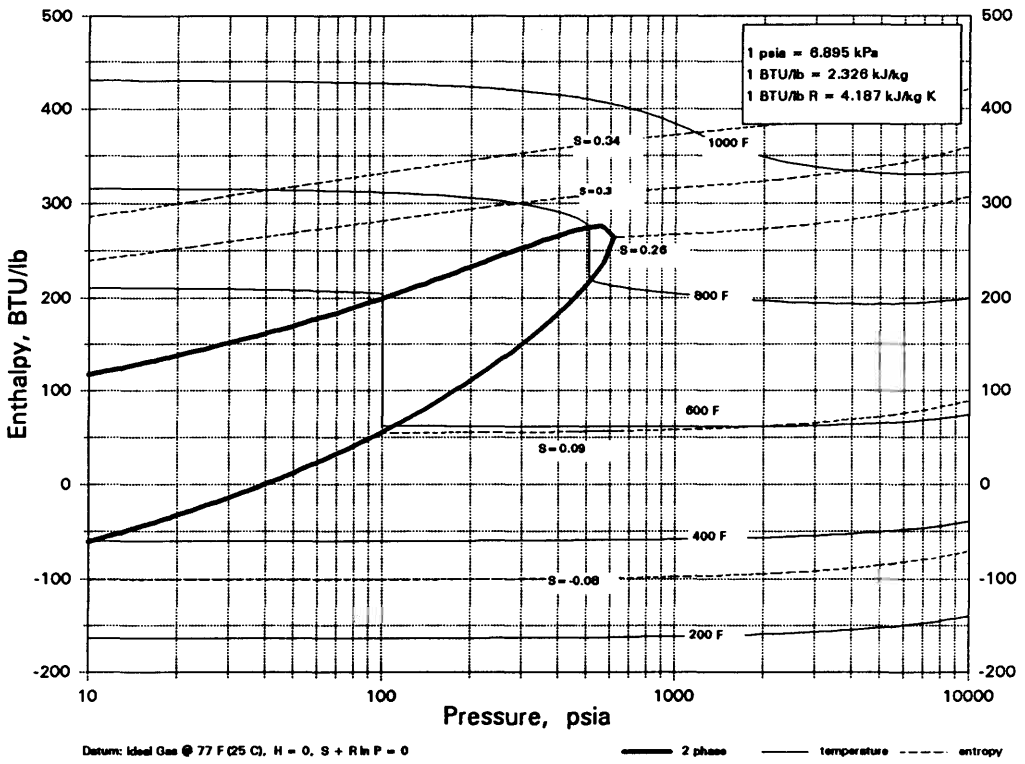
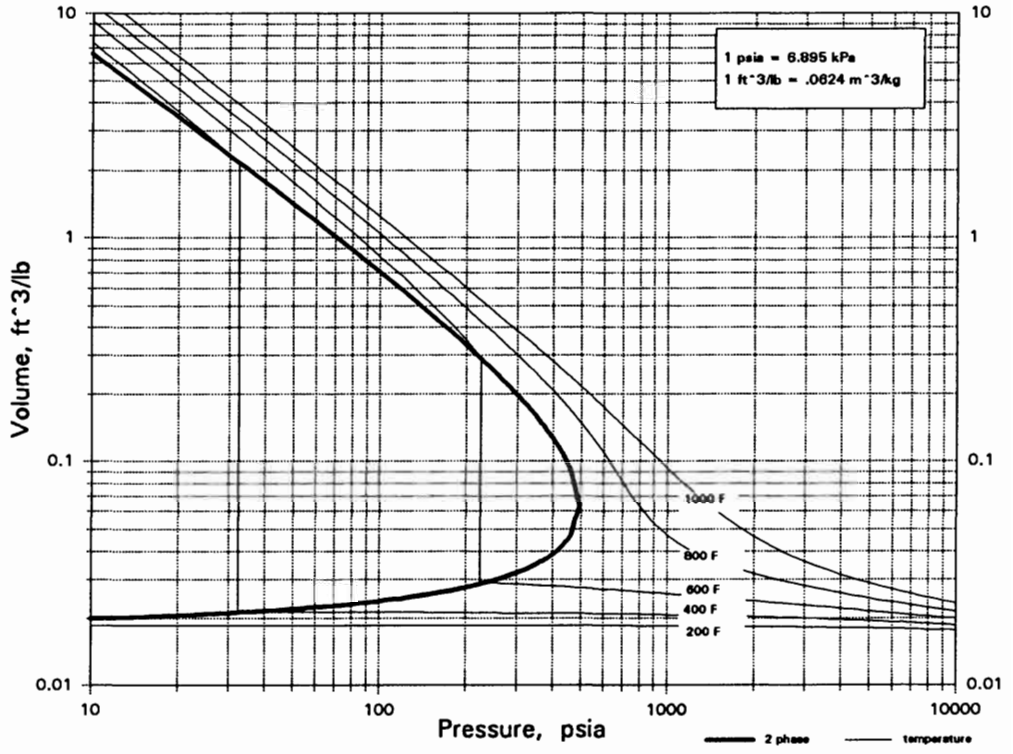
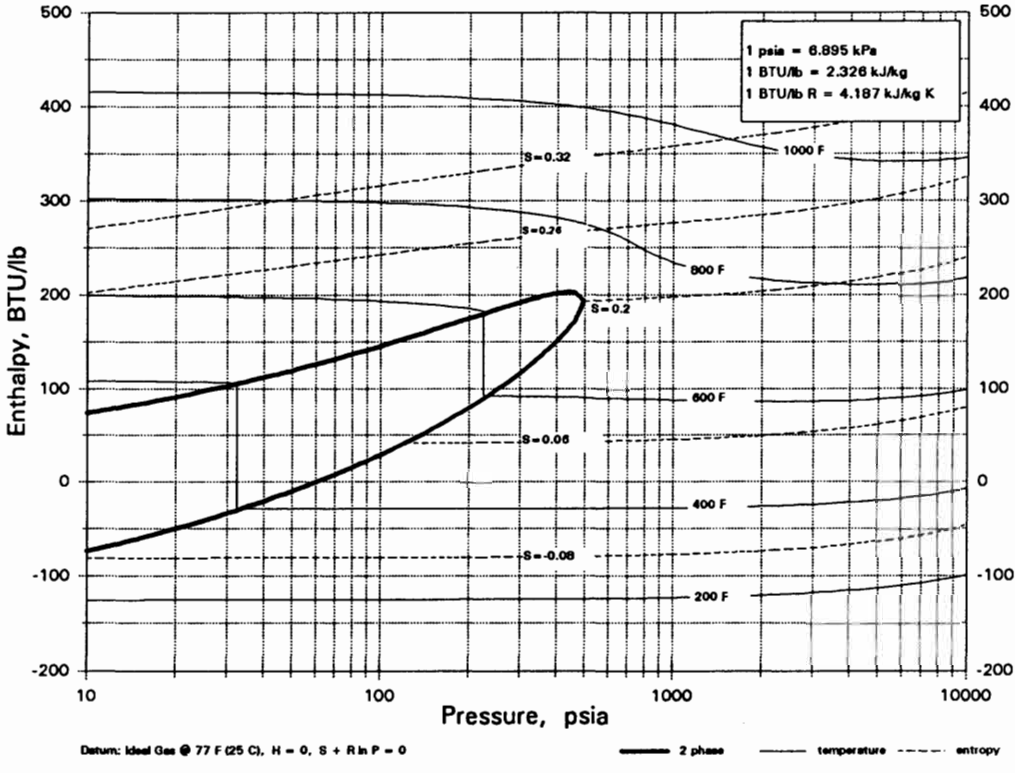


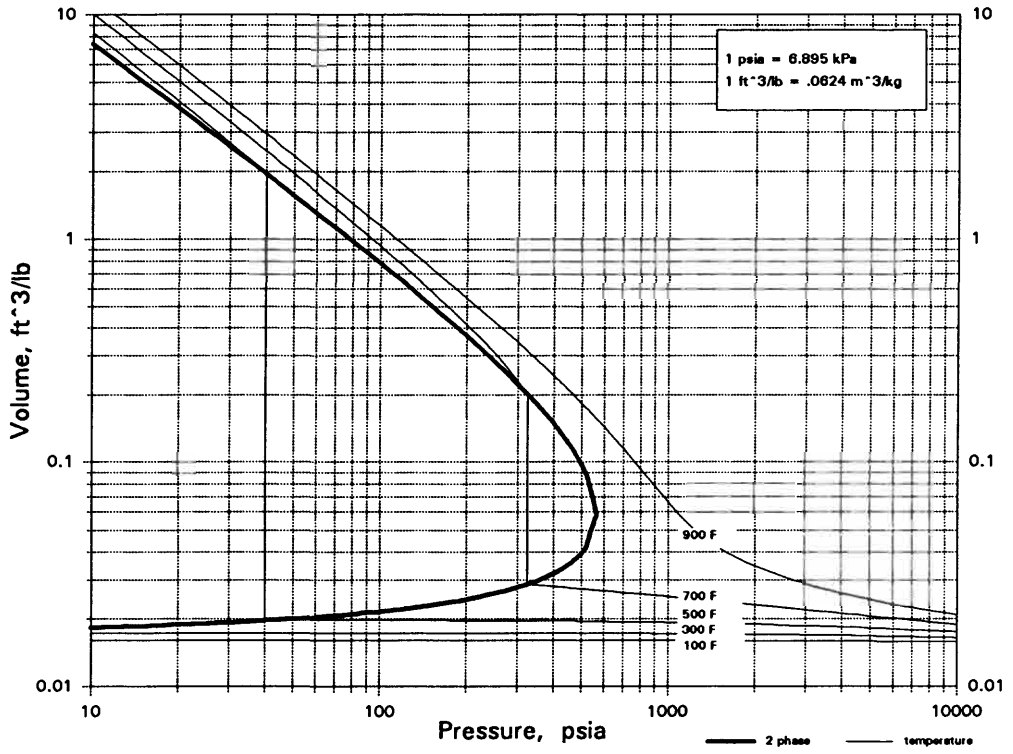


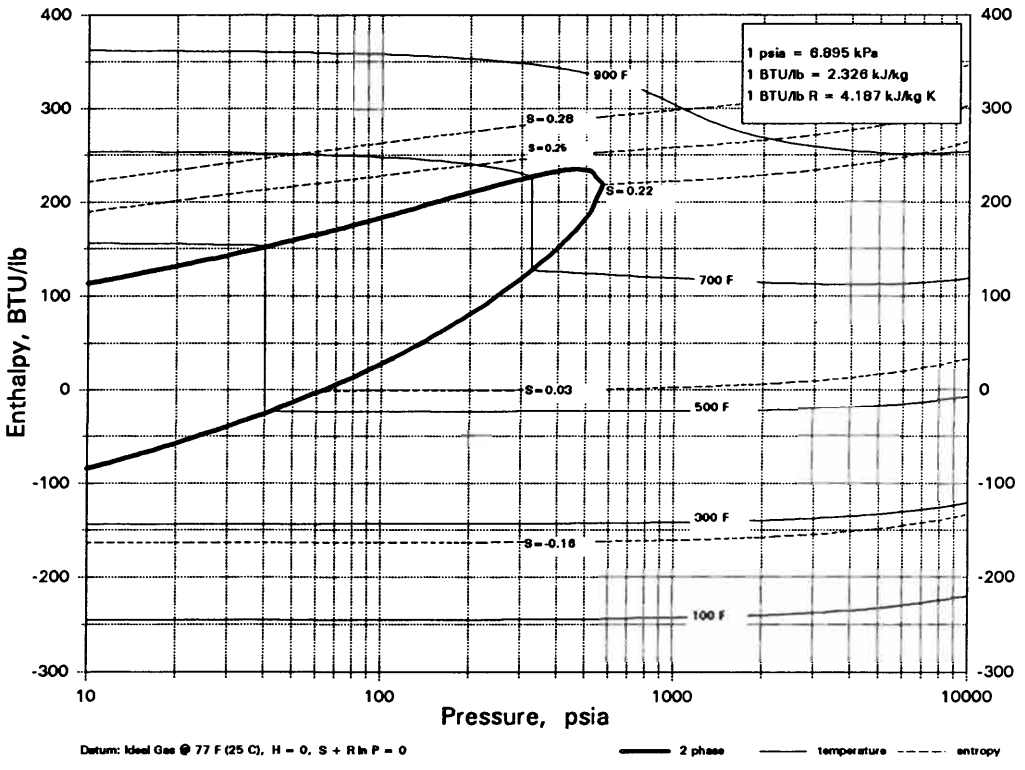
C8H10O PHENETOLE



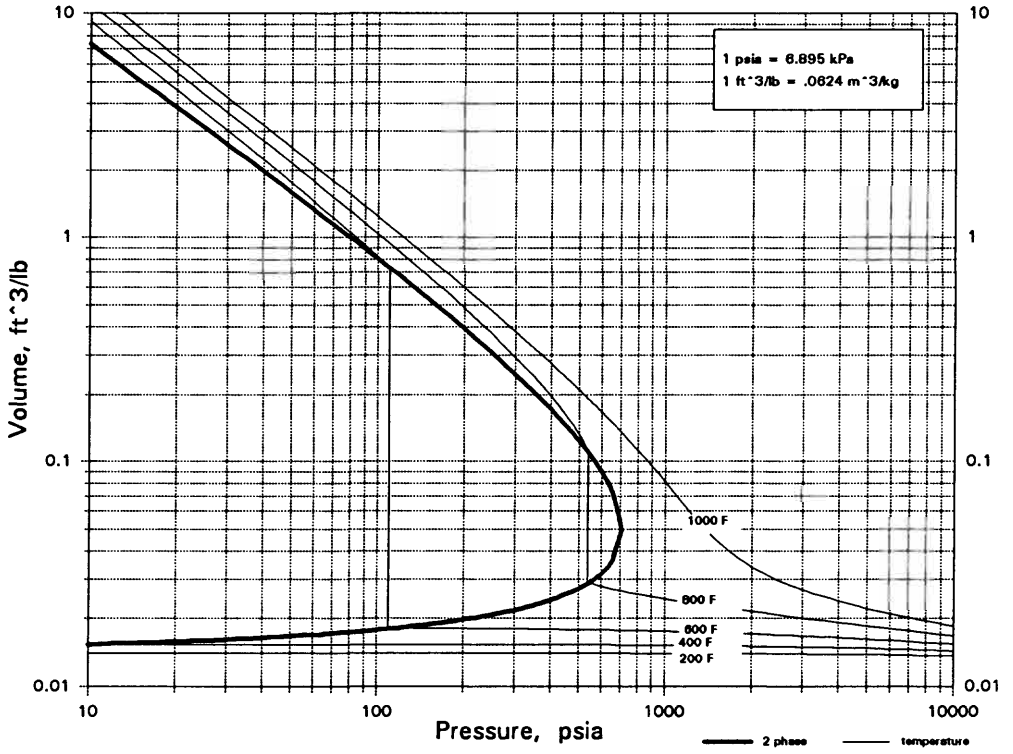


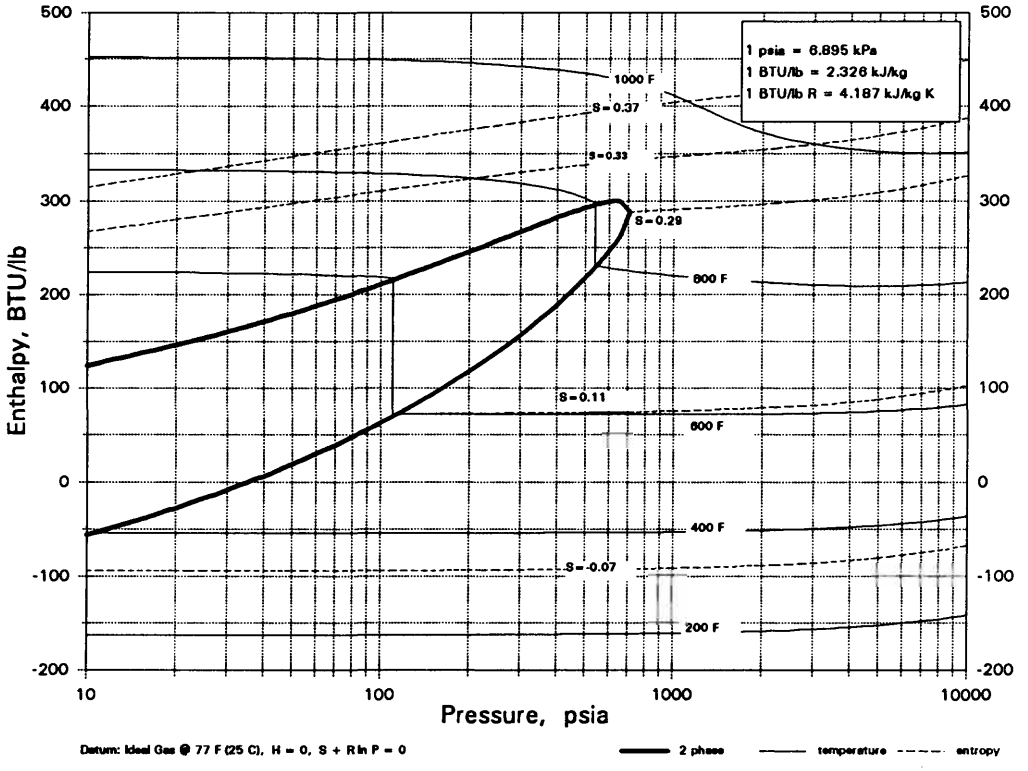
C8H10O 2-PHENYLETHANOL



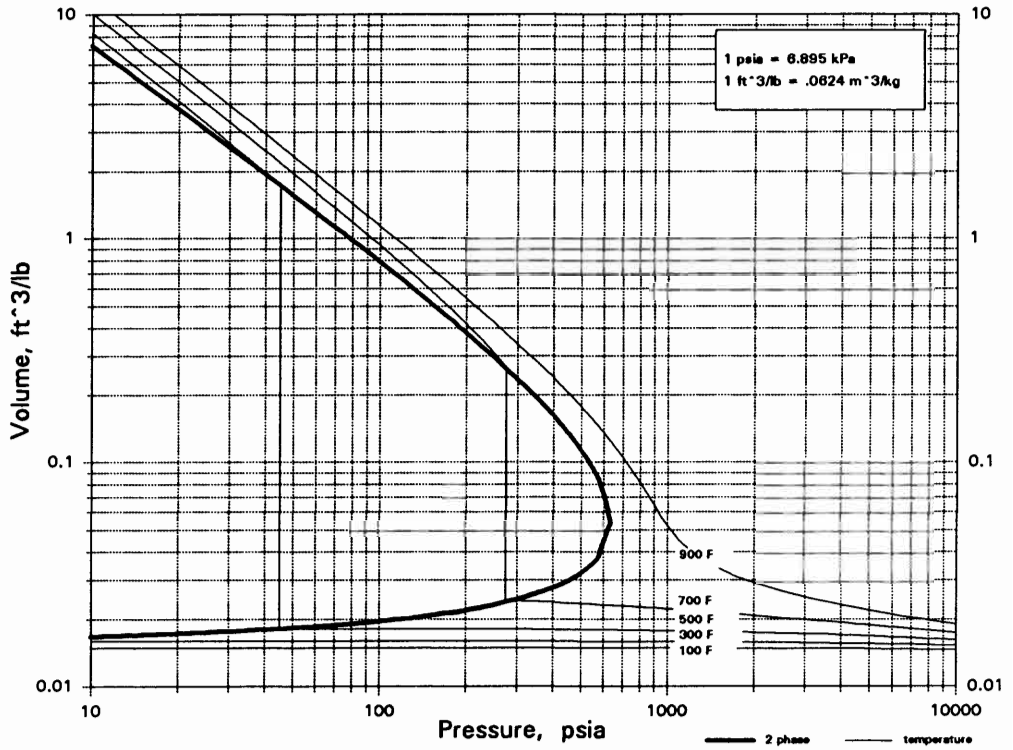


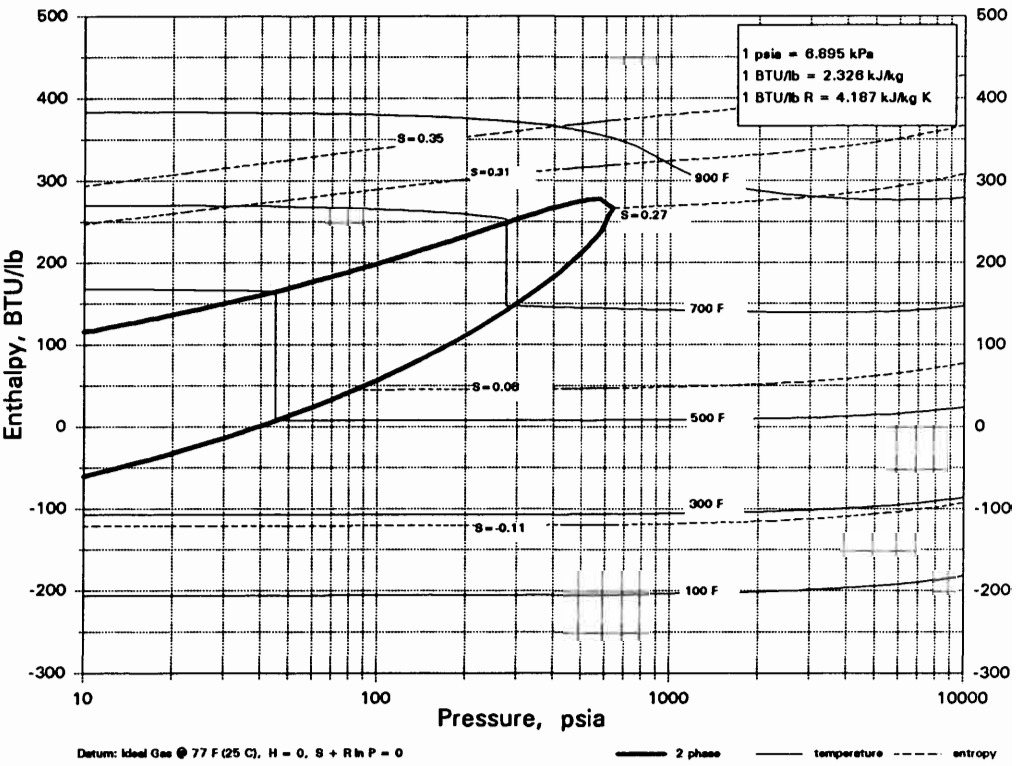
C8H10O 2-3-XYLENOL



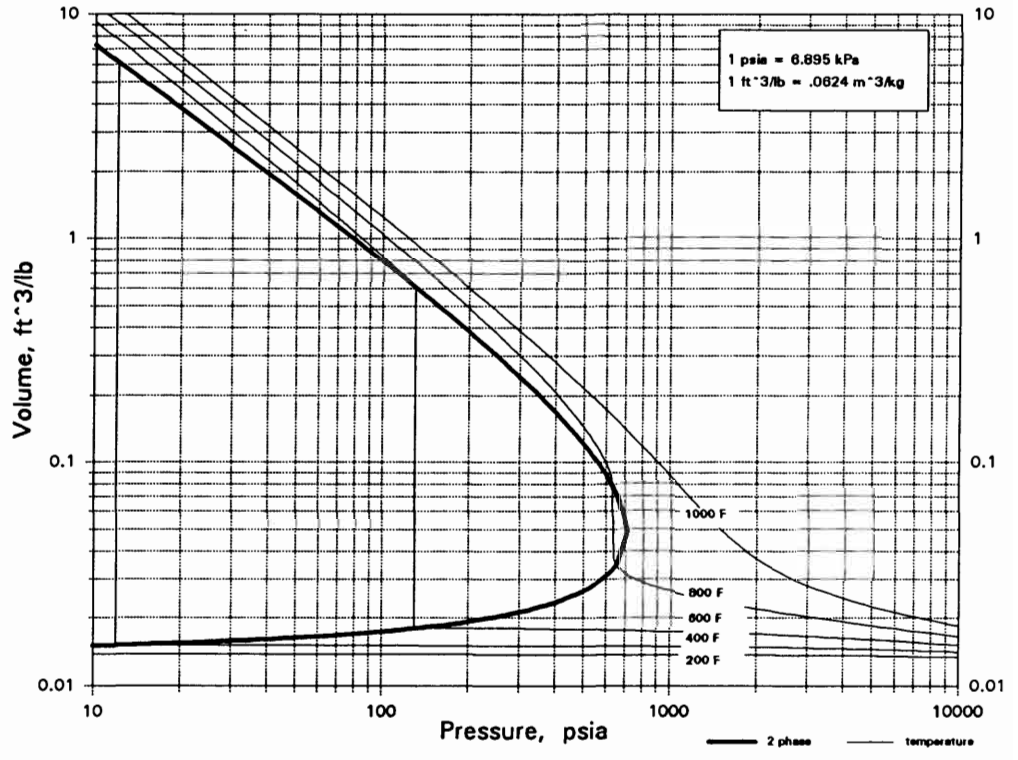


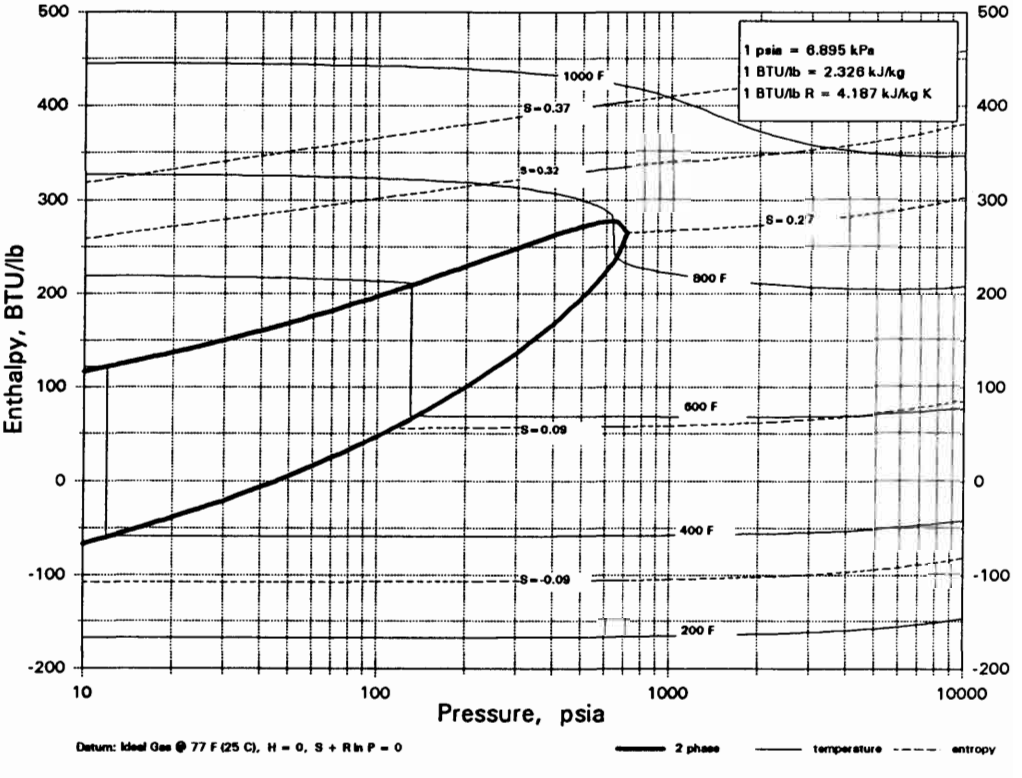
C8H10O 2-4-XYLENOL



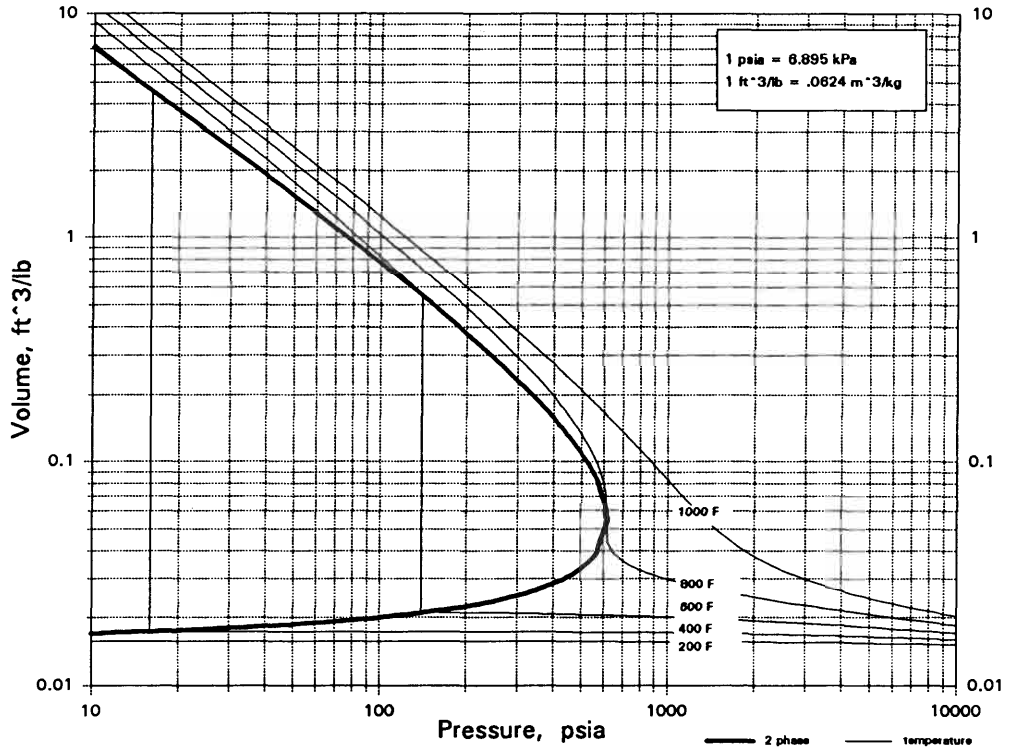


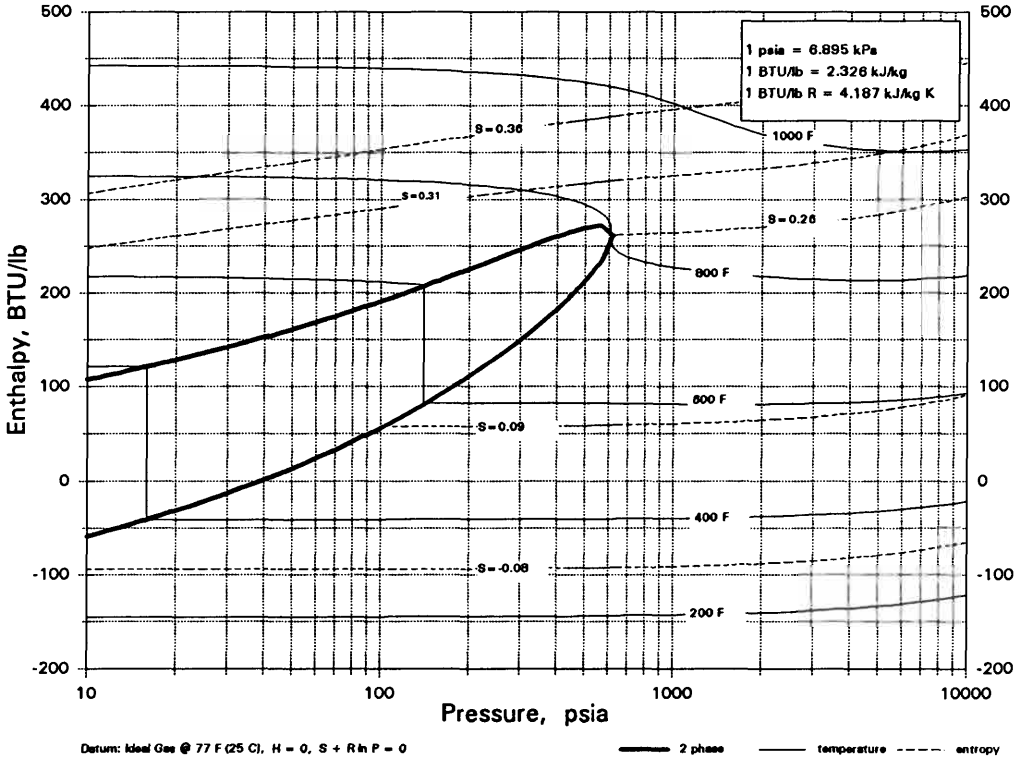
C8H10O 2-5-XYLENOL



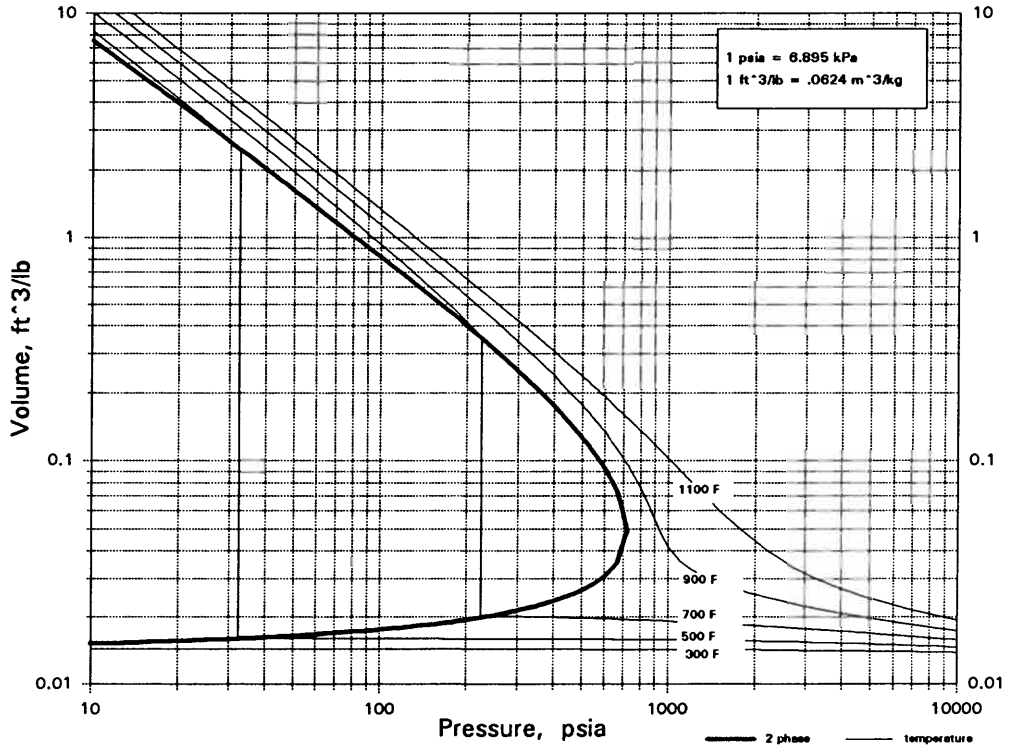


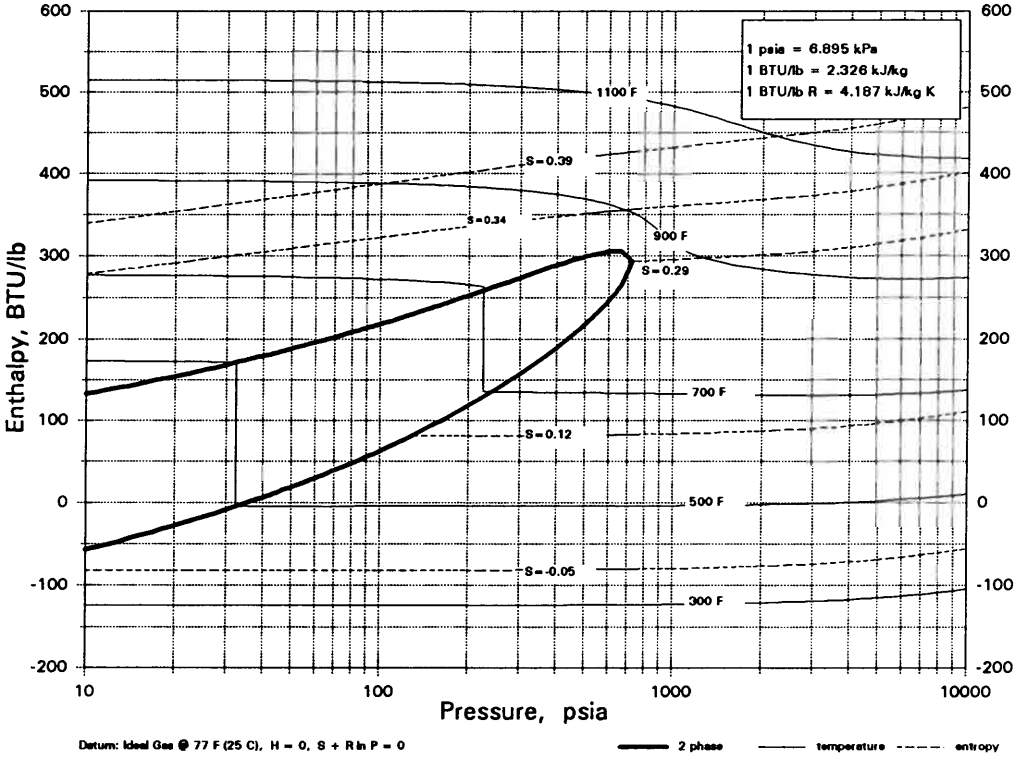
C8H10O 2-6-XYLENOL



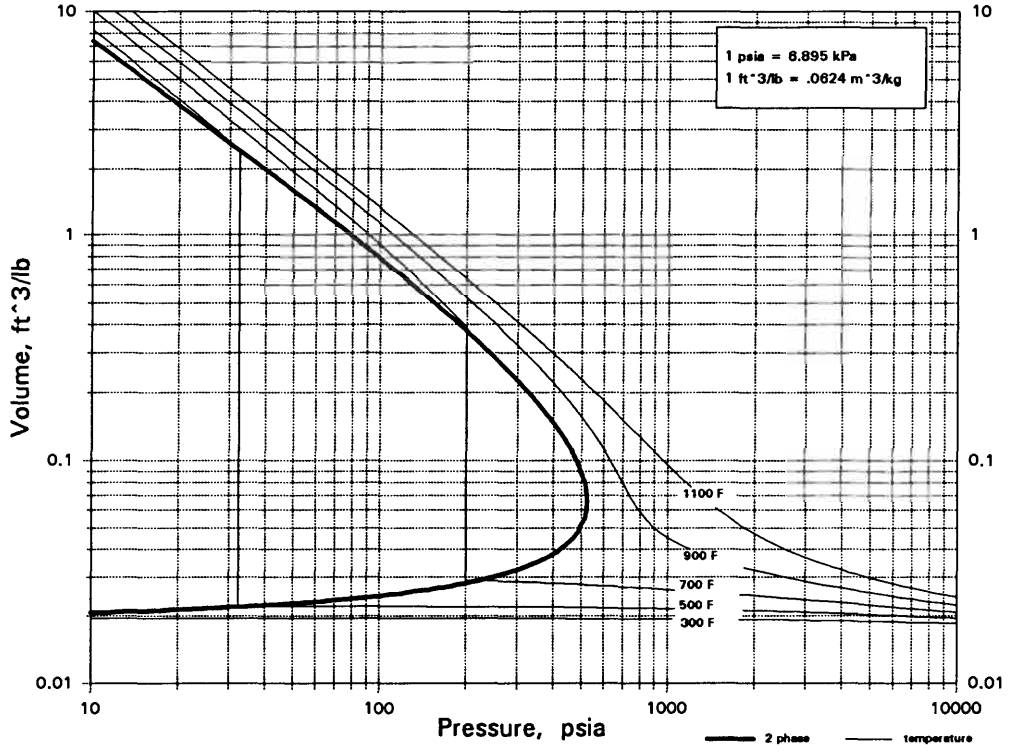


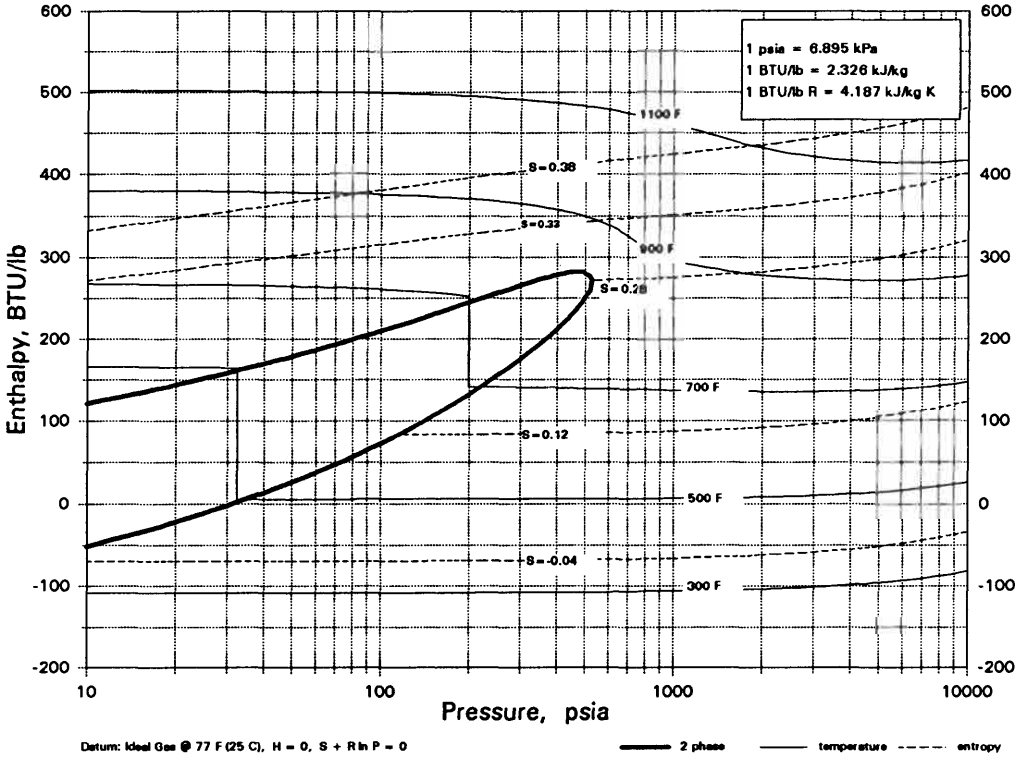
C8H10O 3-4-XYLENOL



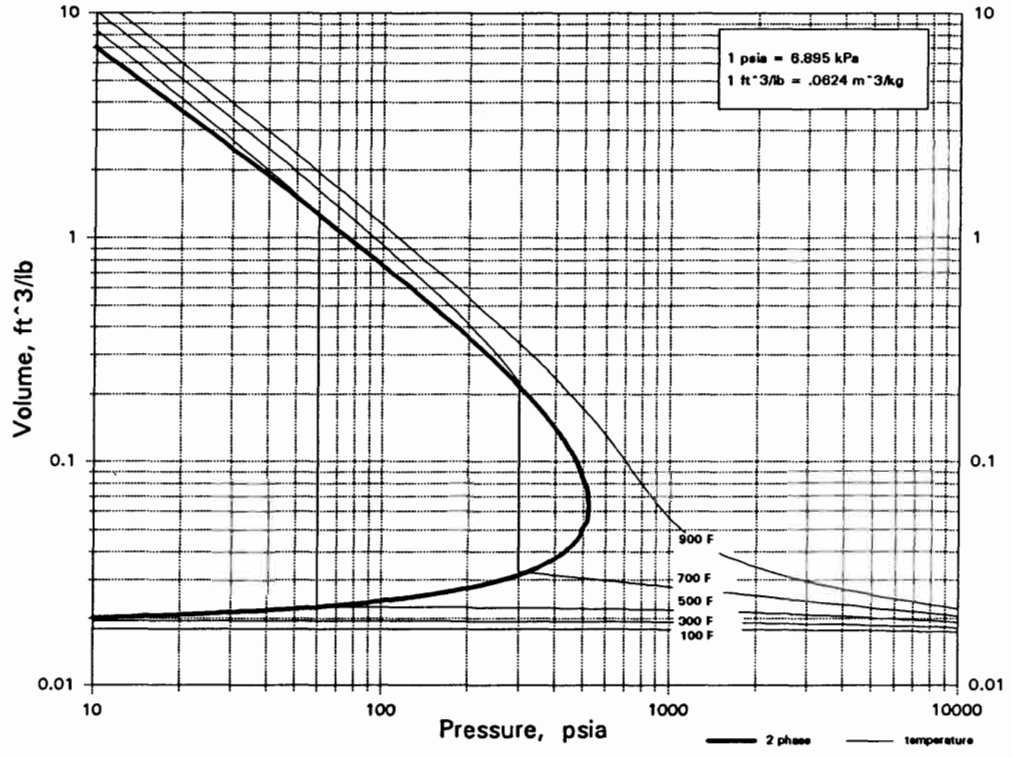


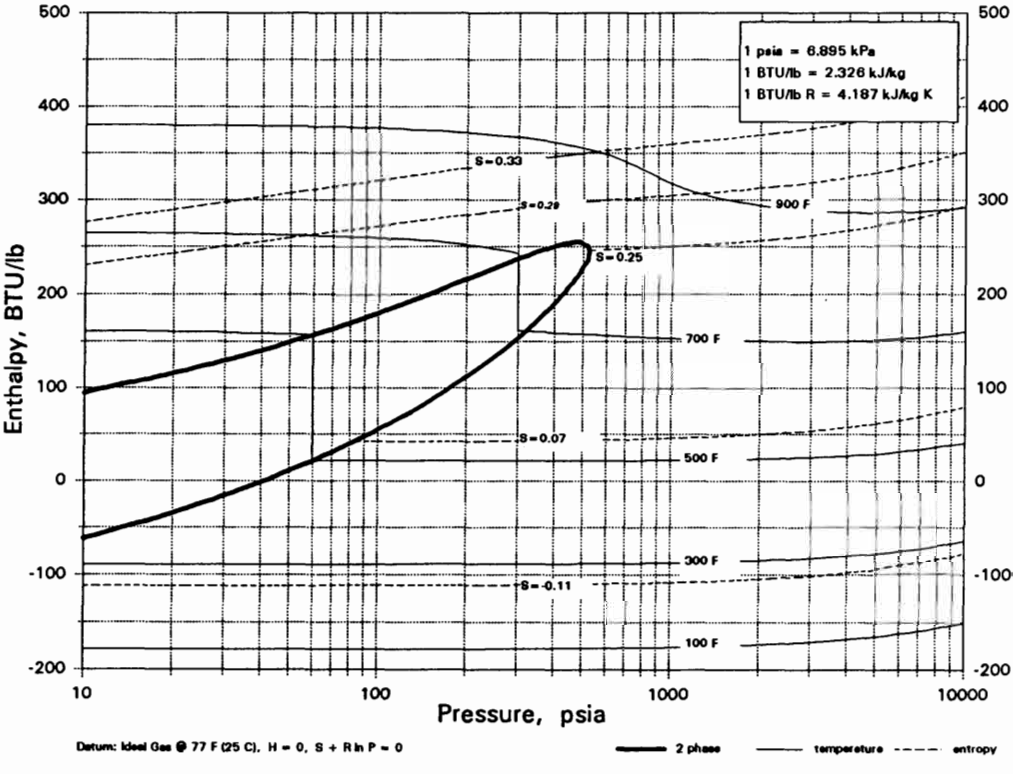
C8H10O 3-5-XYLENOL



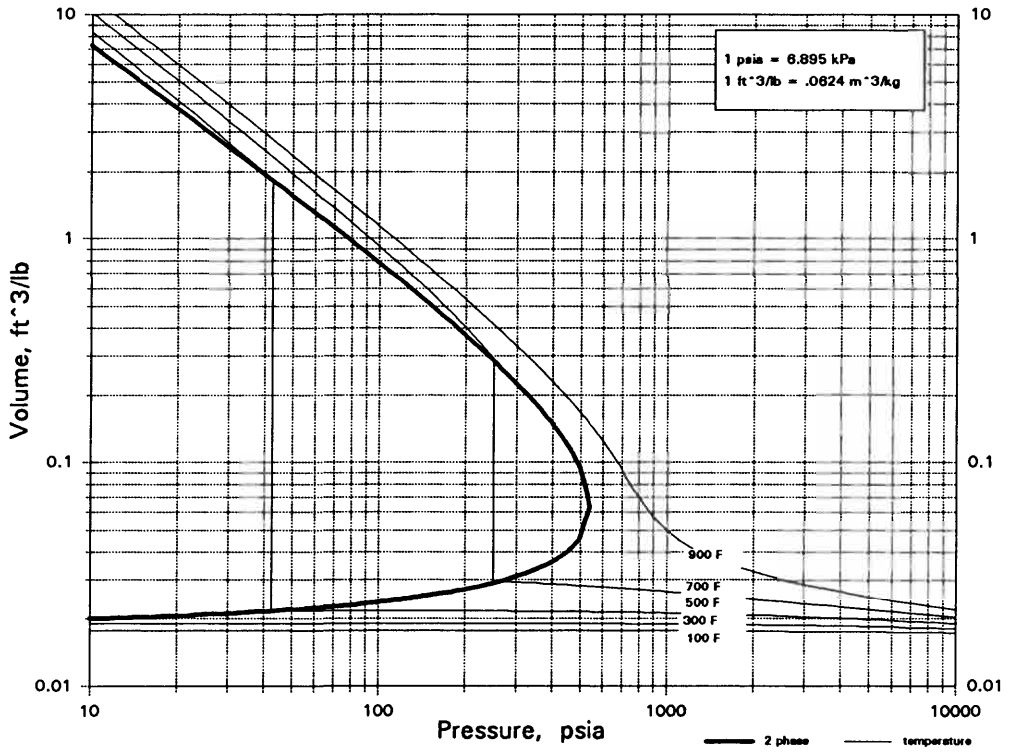


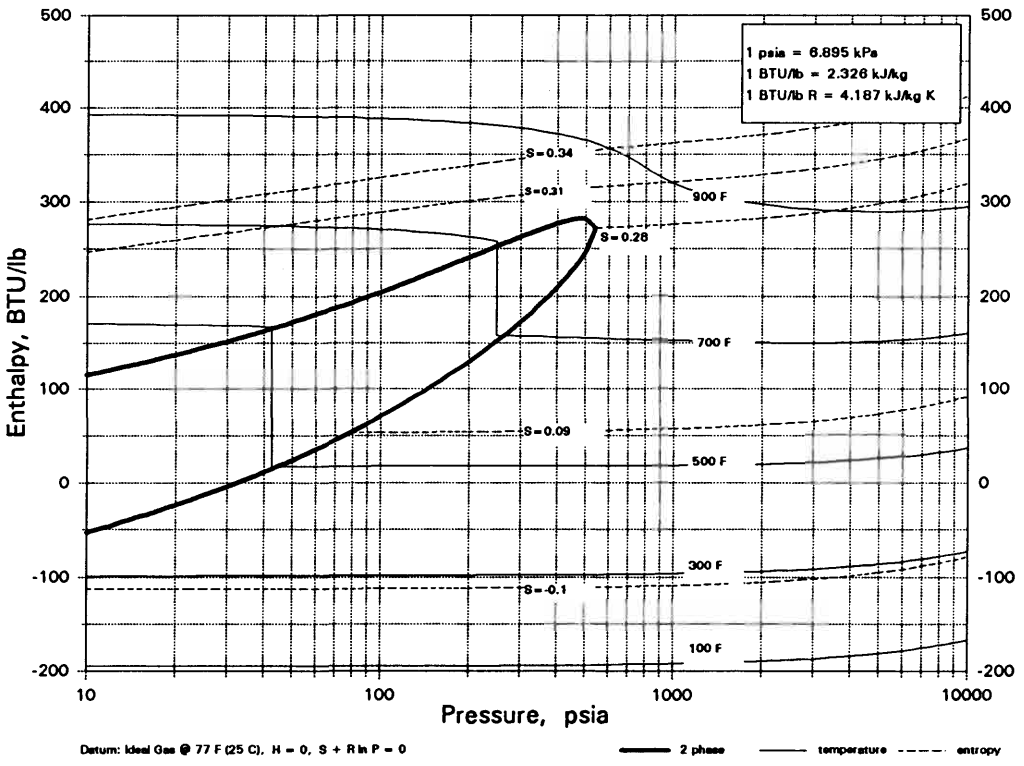
C8H11N N-N-DIMETHYLANILINE



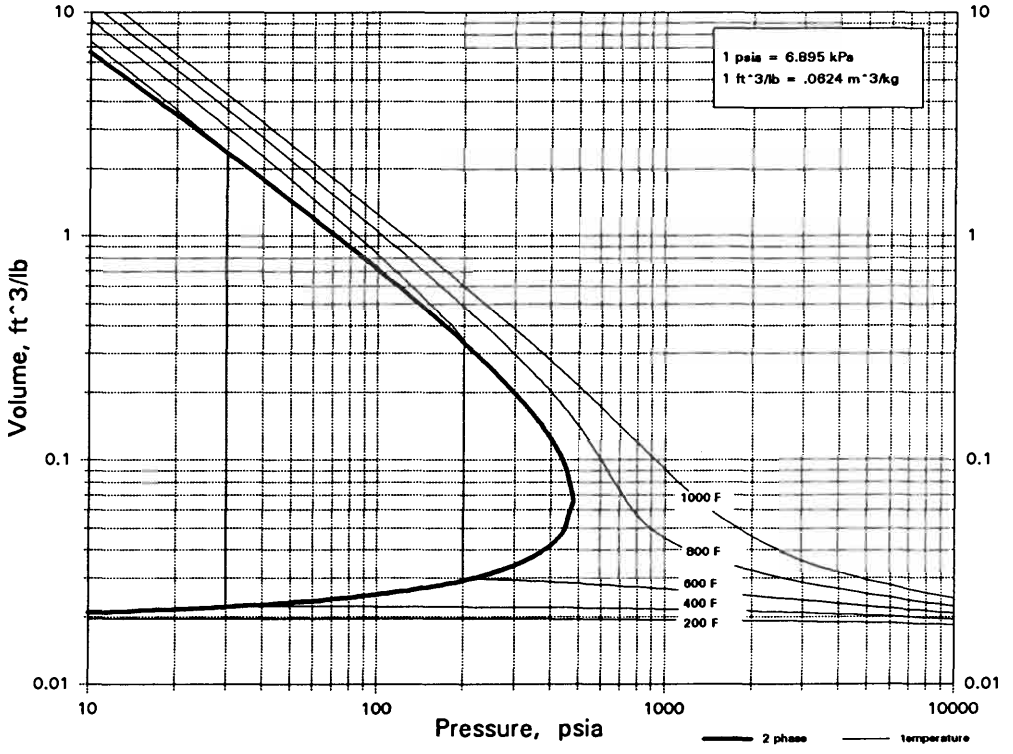


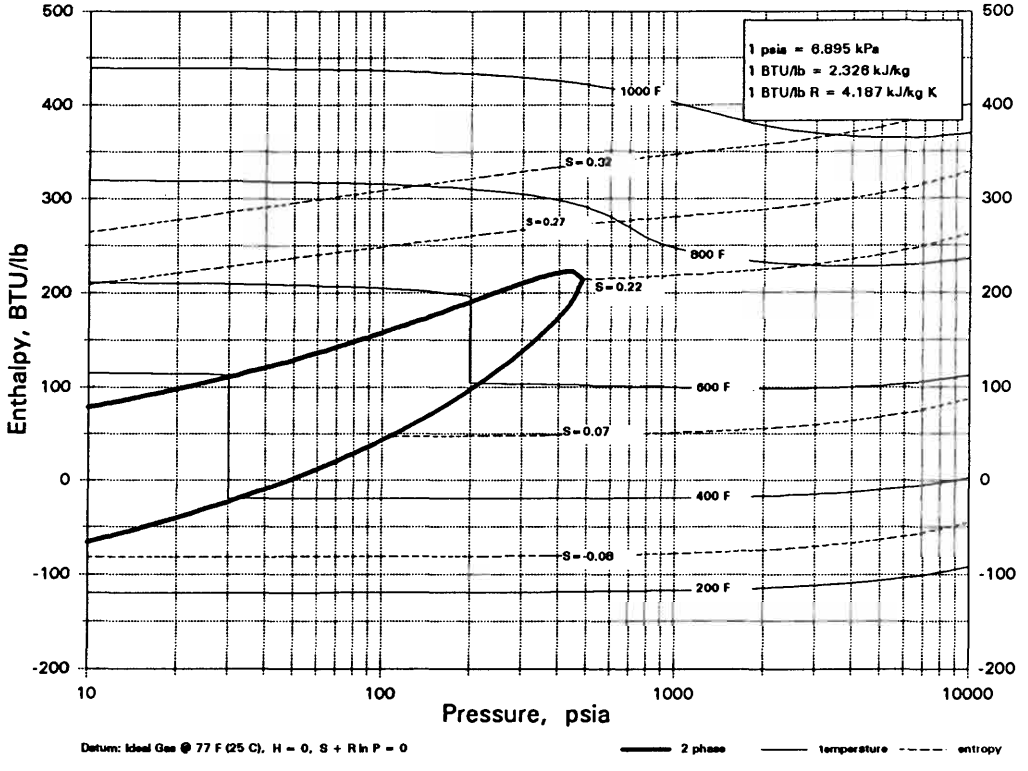
C8H11N o-ETHYLANILINE



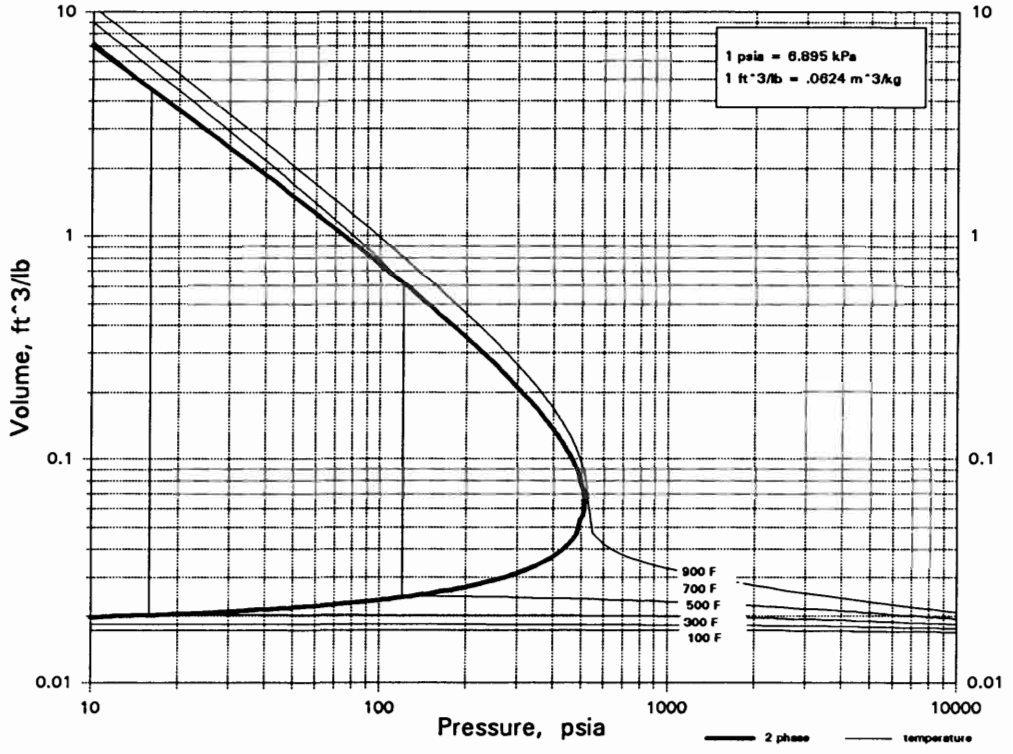


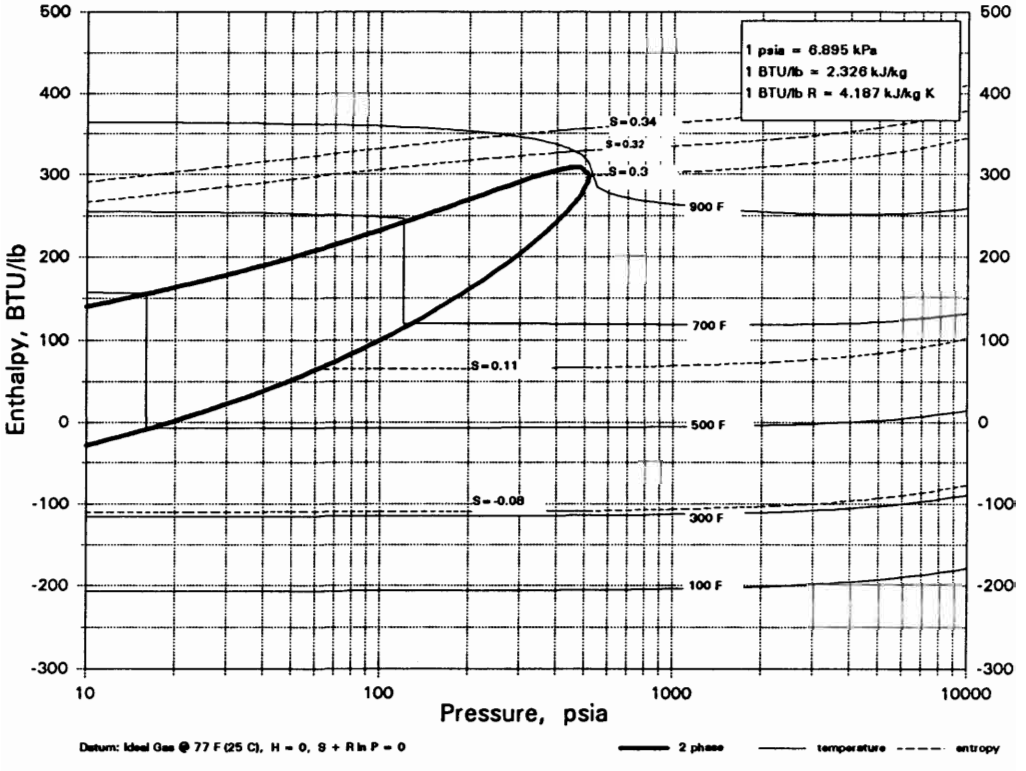
C8H11N 2-4-6-TRIMETHYLPYRIDINE



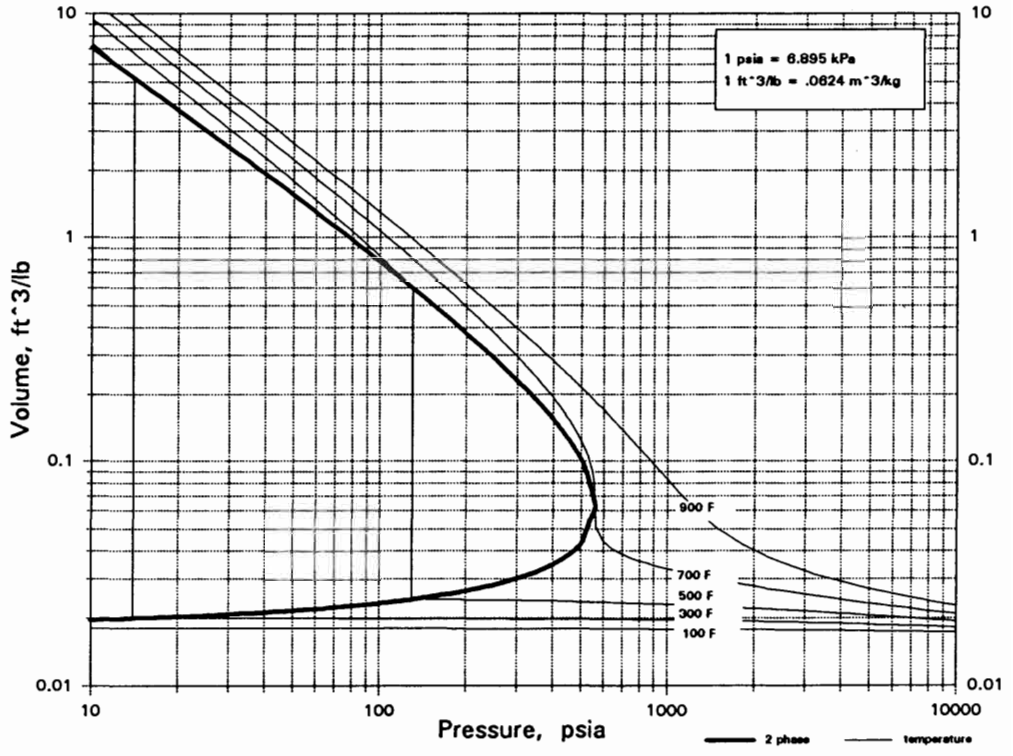


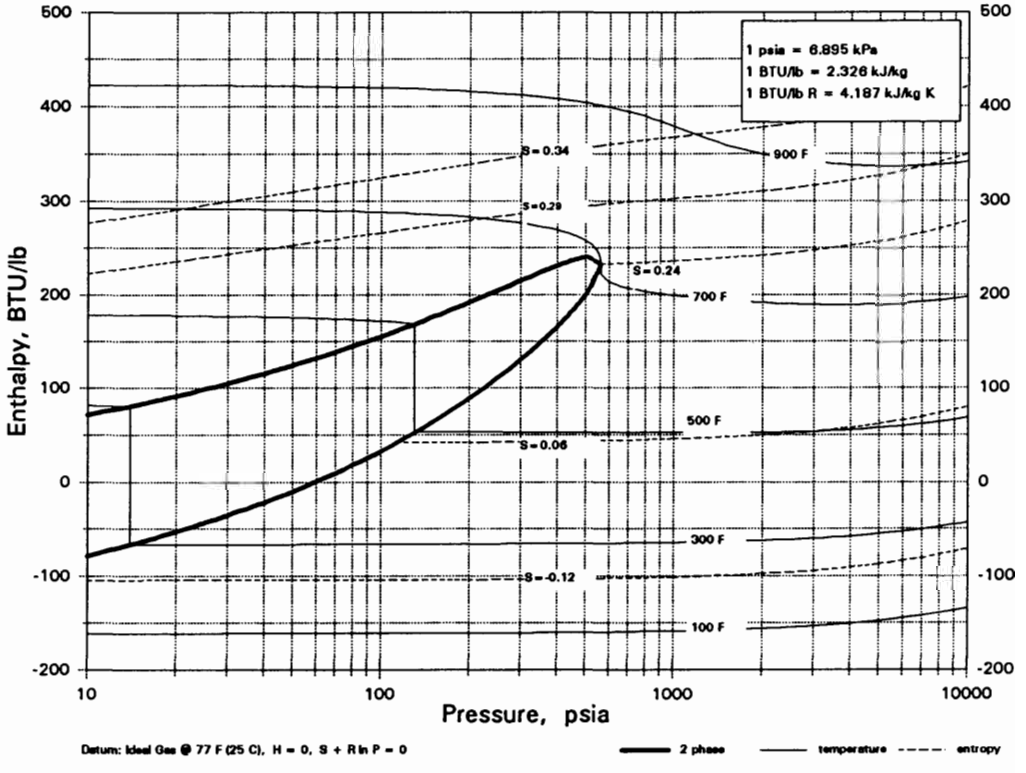
C8H11NO p-PHENETIDINE



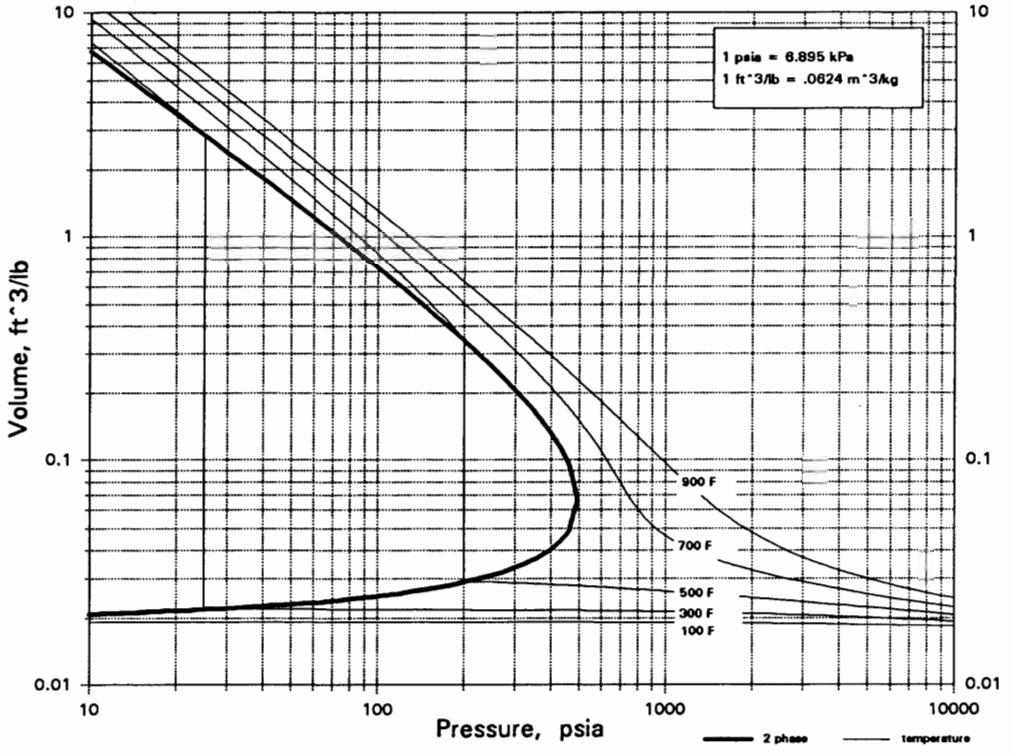


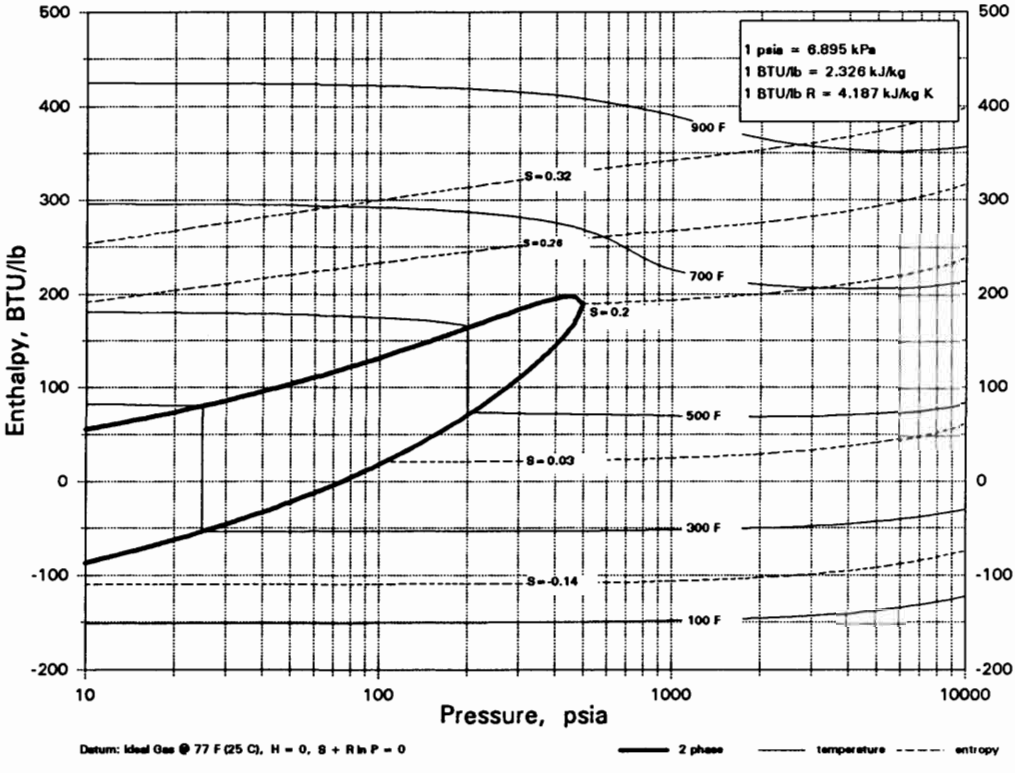
C8H12 1-5-CYCLOOCTADIENE



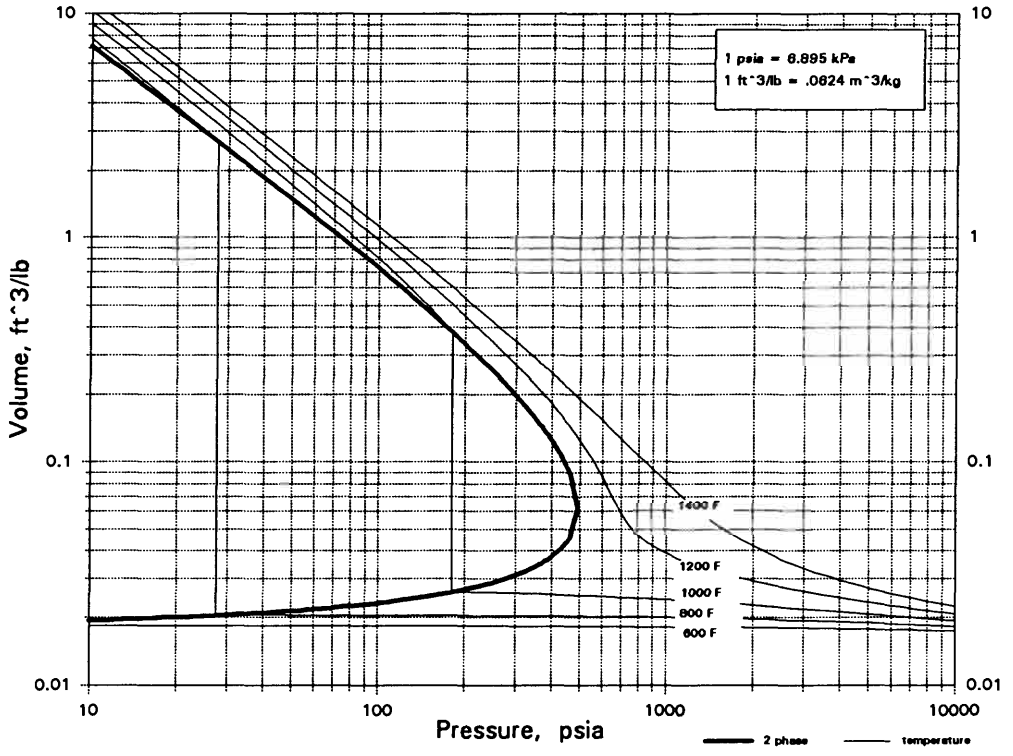


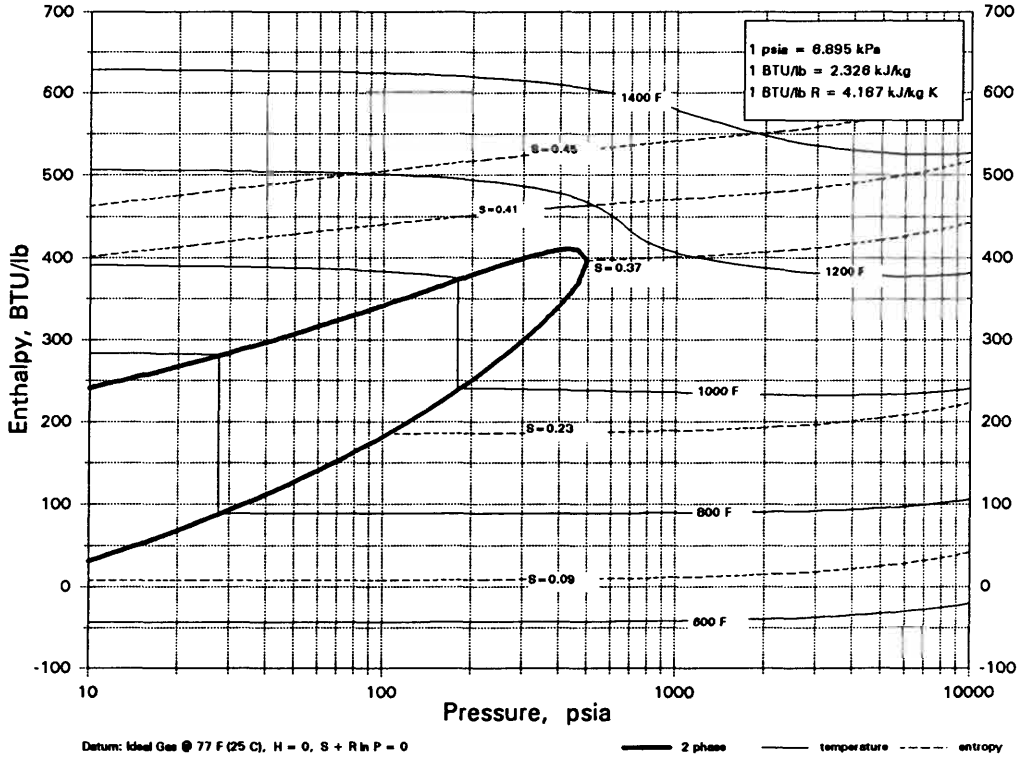
C8H12 VINYLCYCLOHEXENE



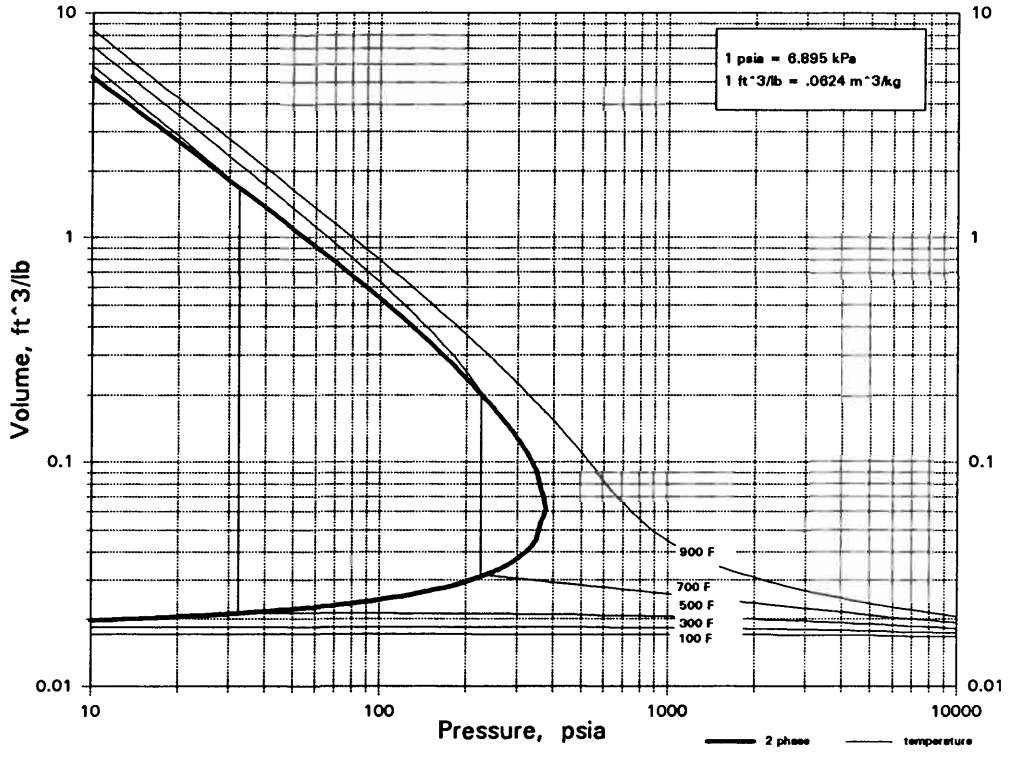


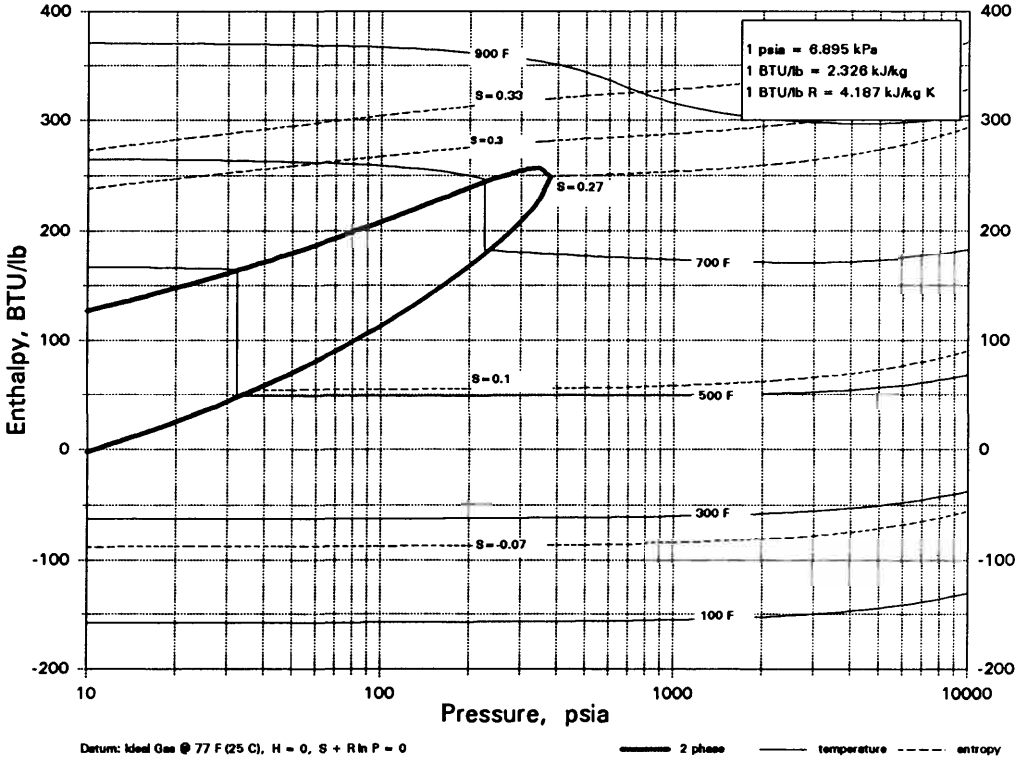
C8H12O4	1-4-CYCLOHEXANEDICARBOXYLIC ACID



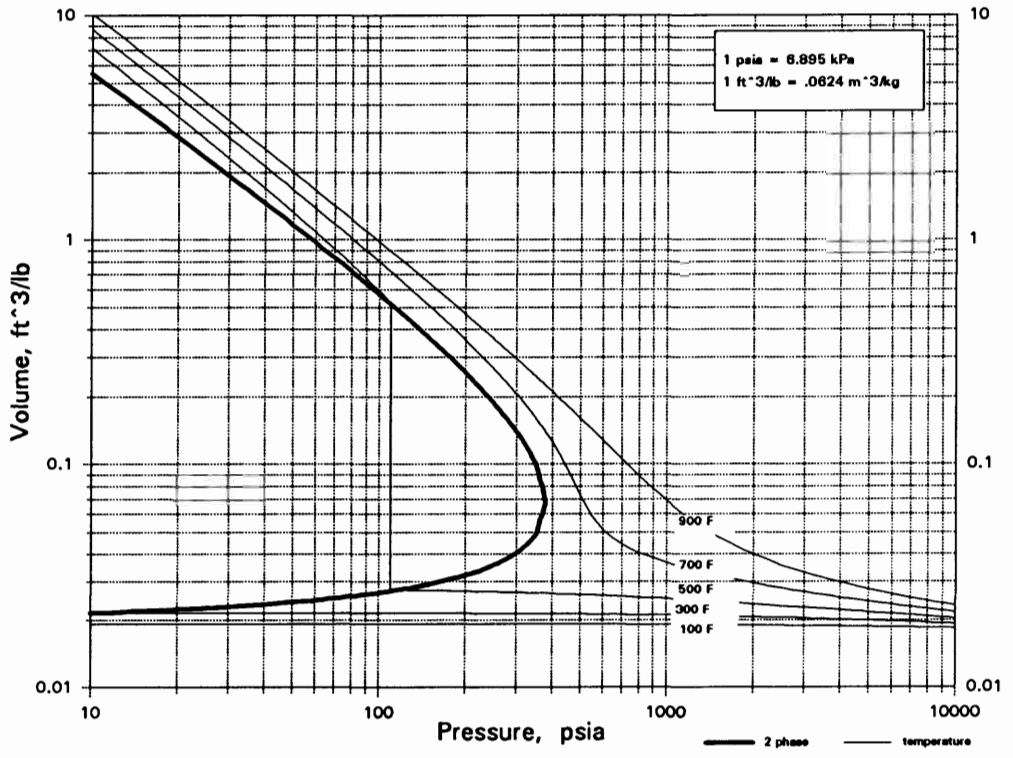


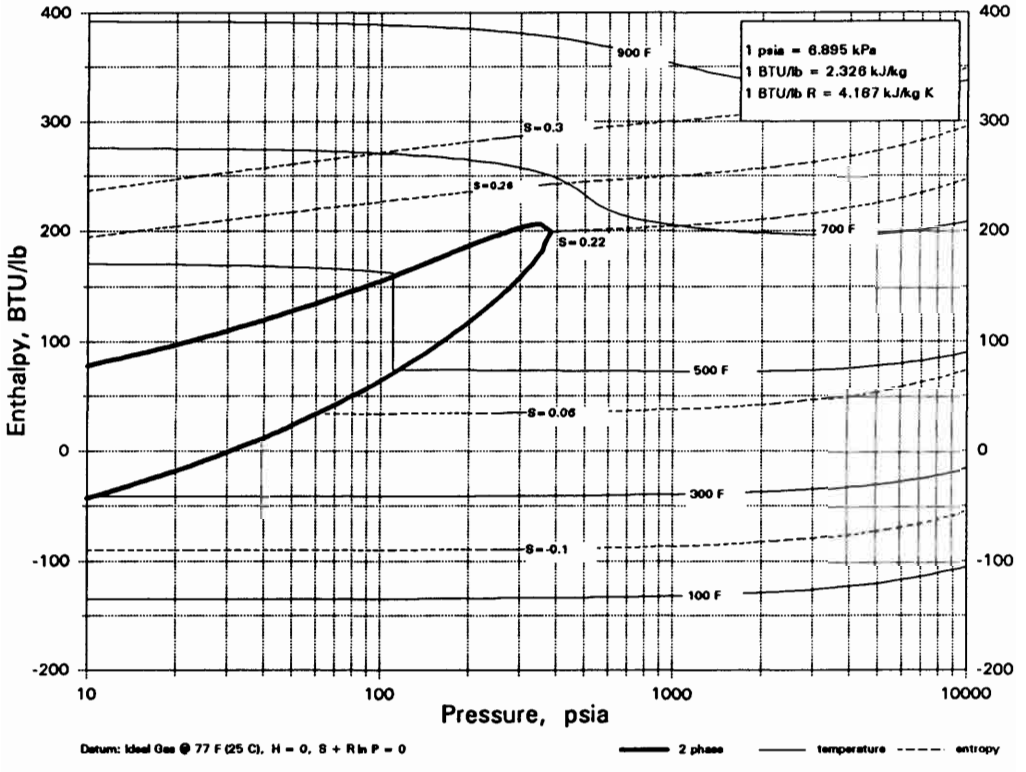
C8H12O4 DIETHYL MALEATE



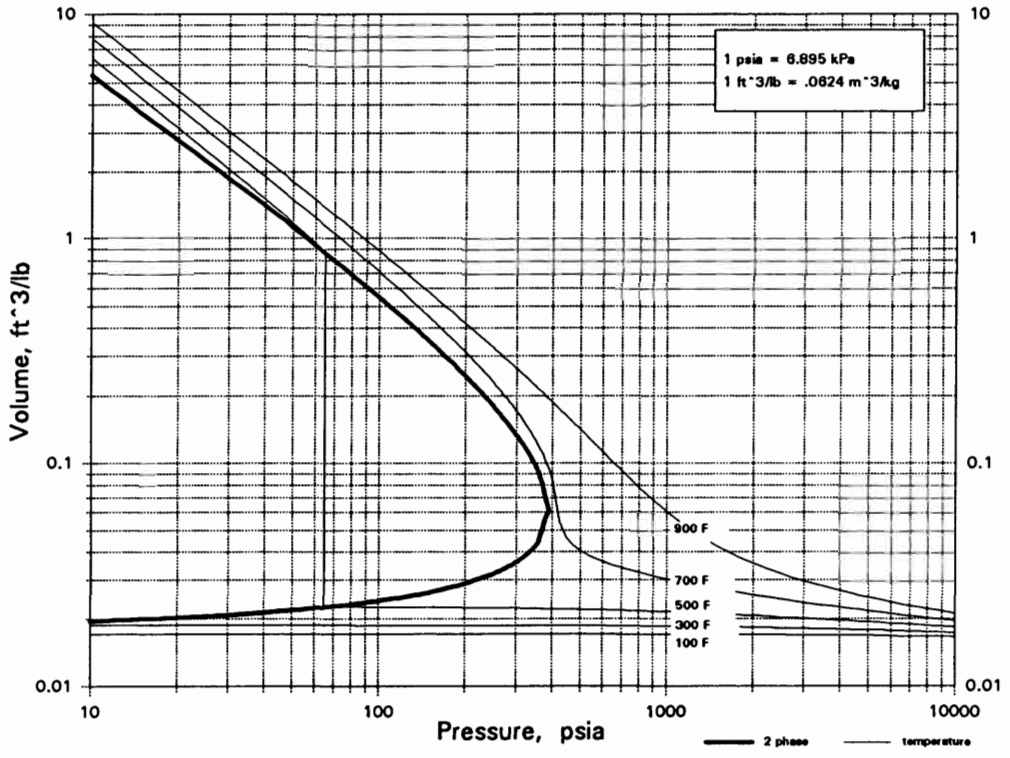


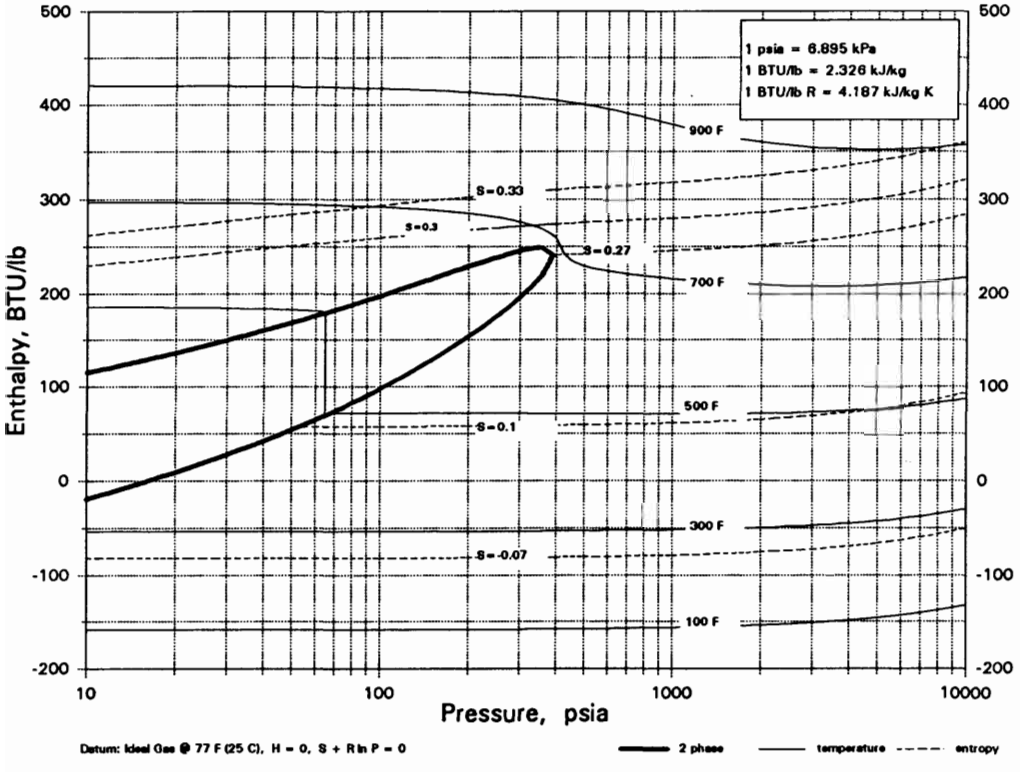
C8H14O2 n-BUTYL METHACRYLATE



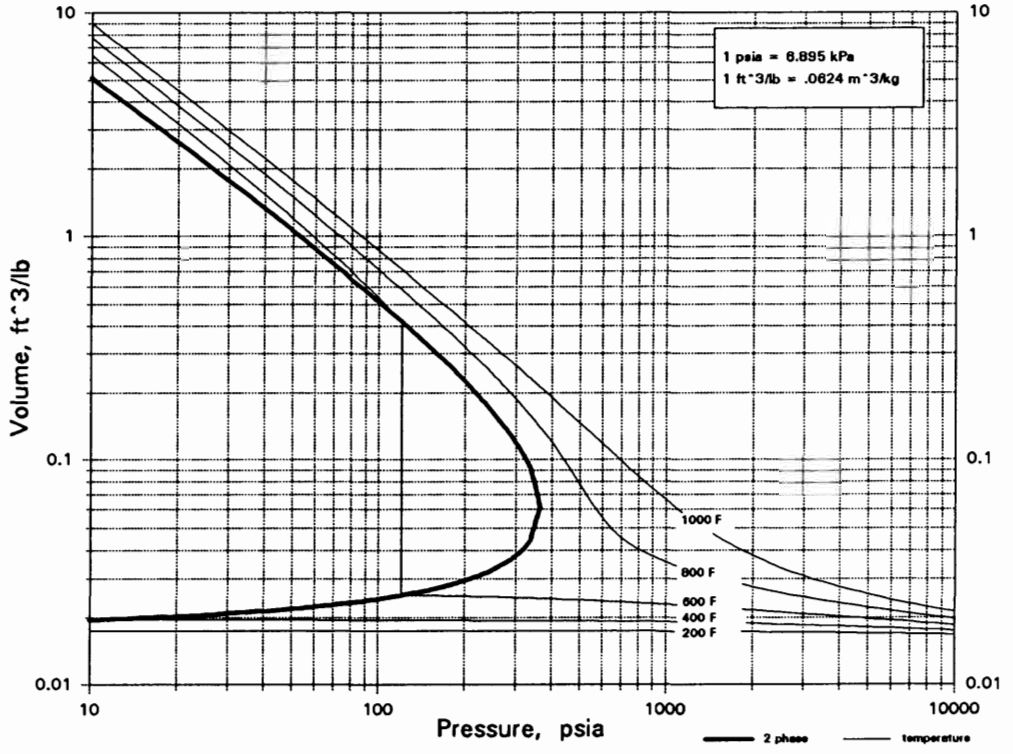


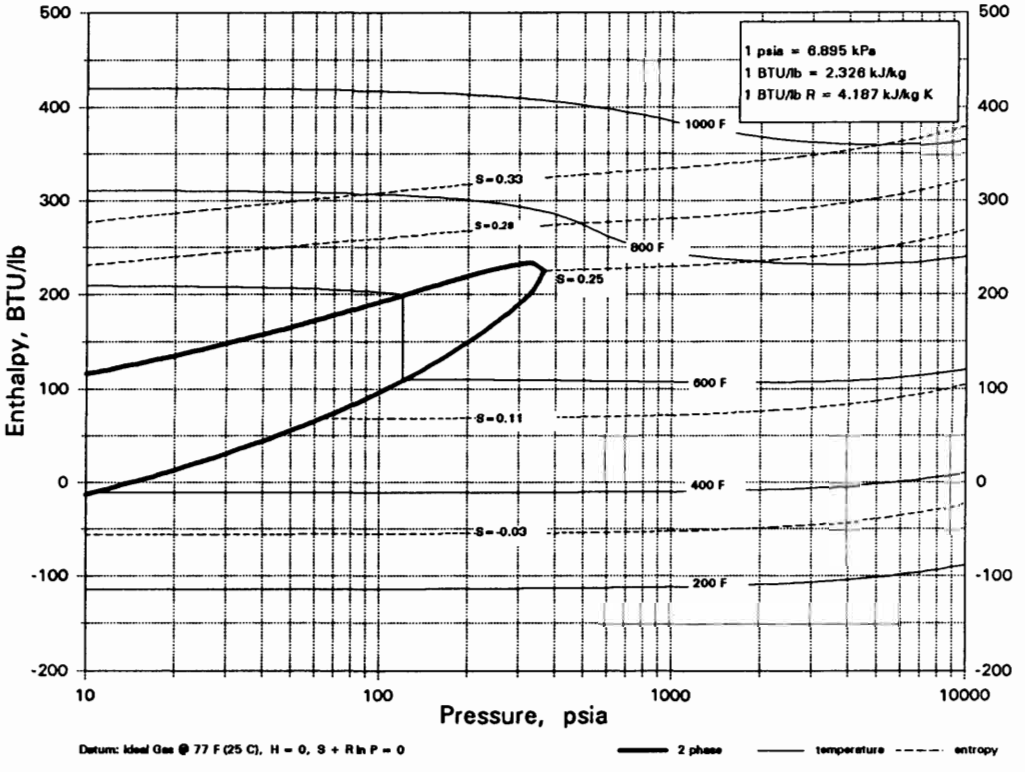
C8H14O3 BUTYRIC ANHYDRIDE



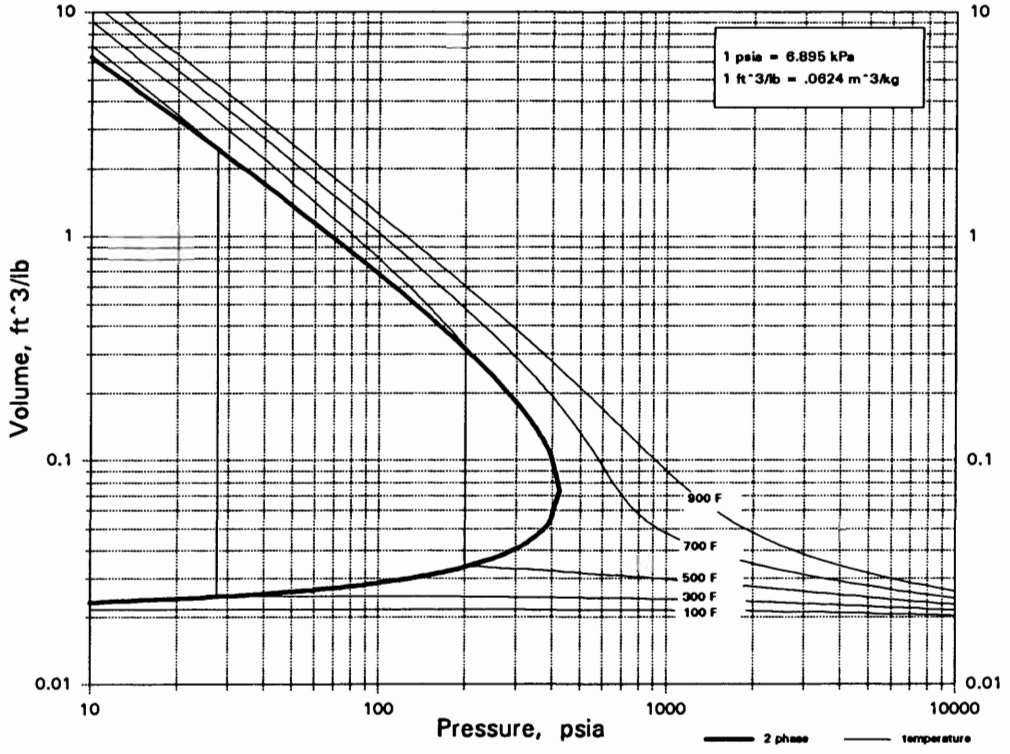


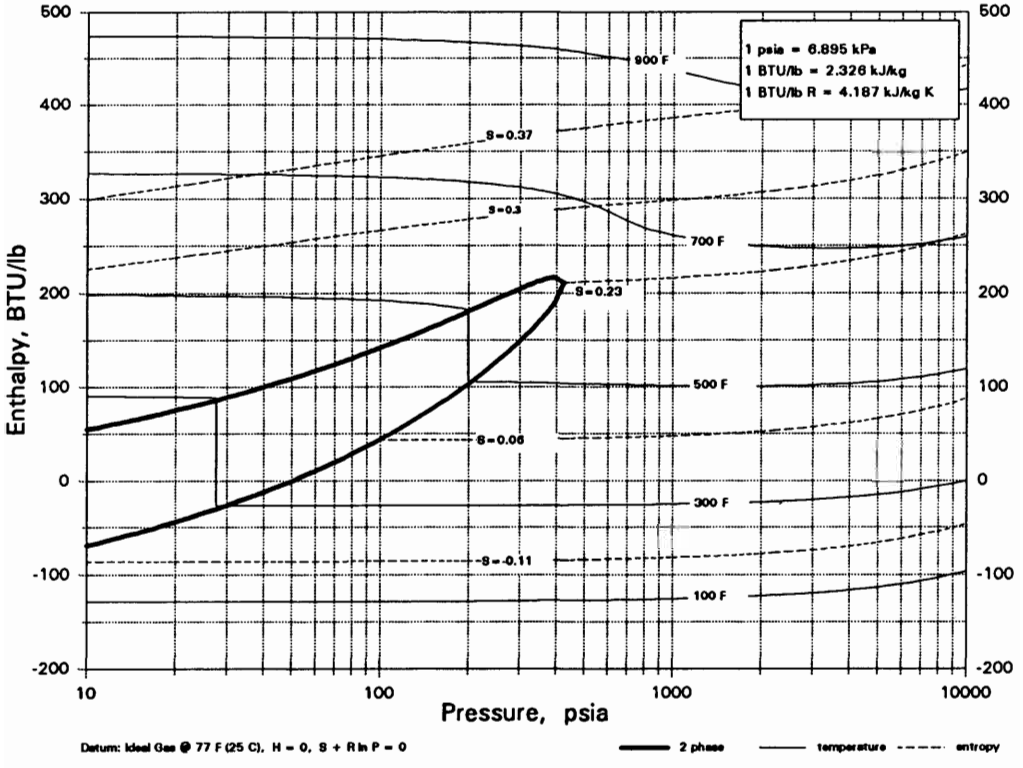
C8H14O4 DIETHYL SUCCINATE



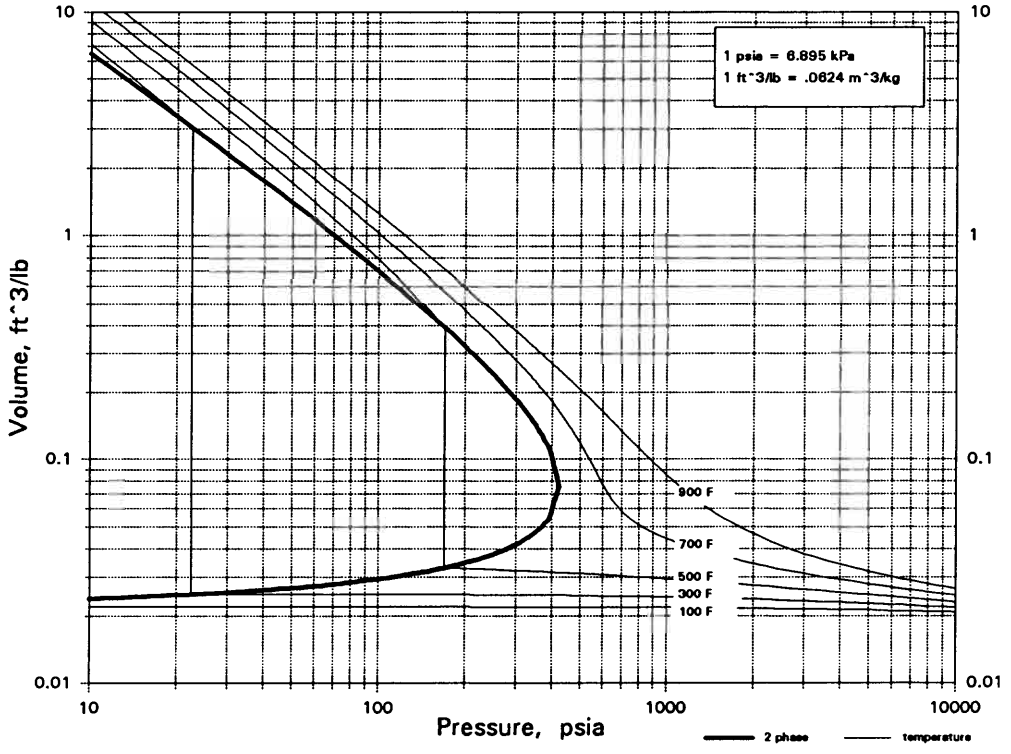


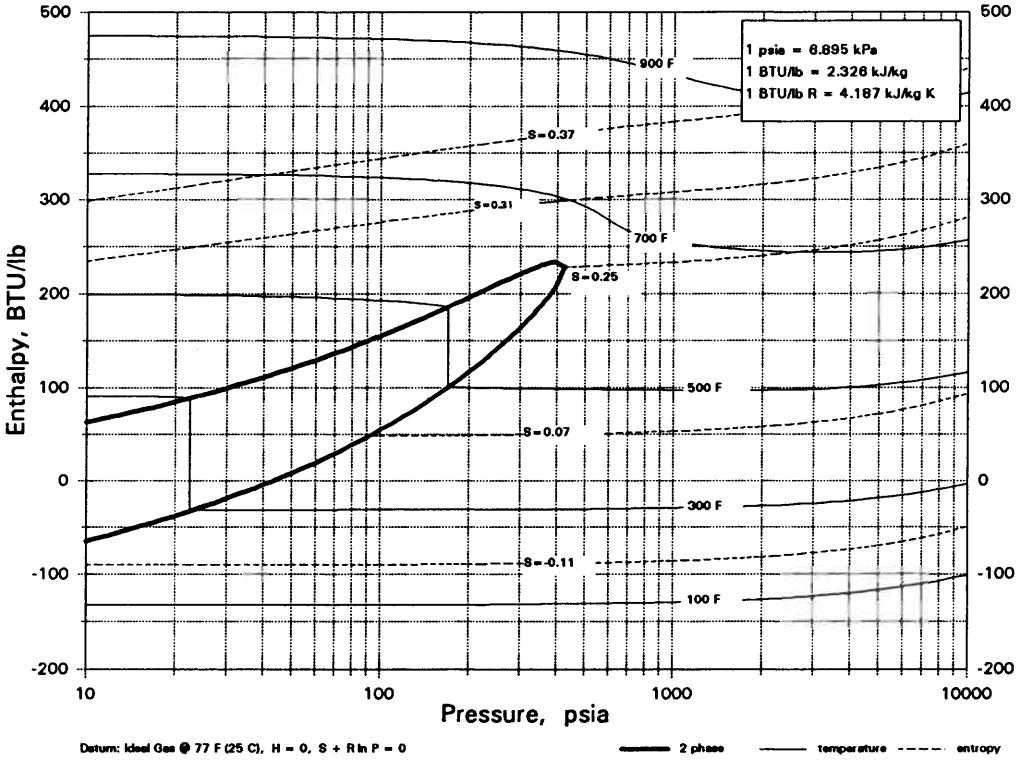
C8H16 1-1-DIMETHYLCYCLOHEXANE



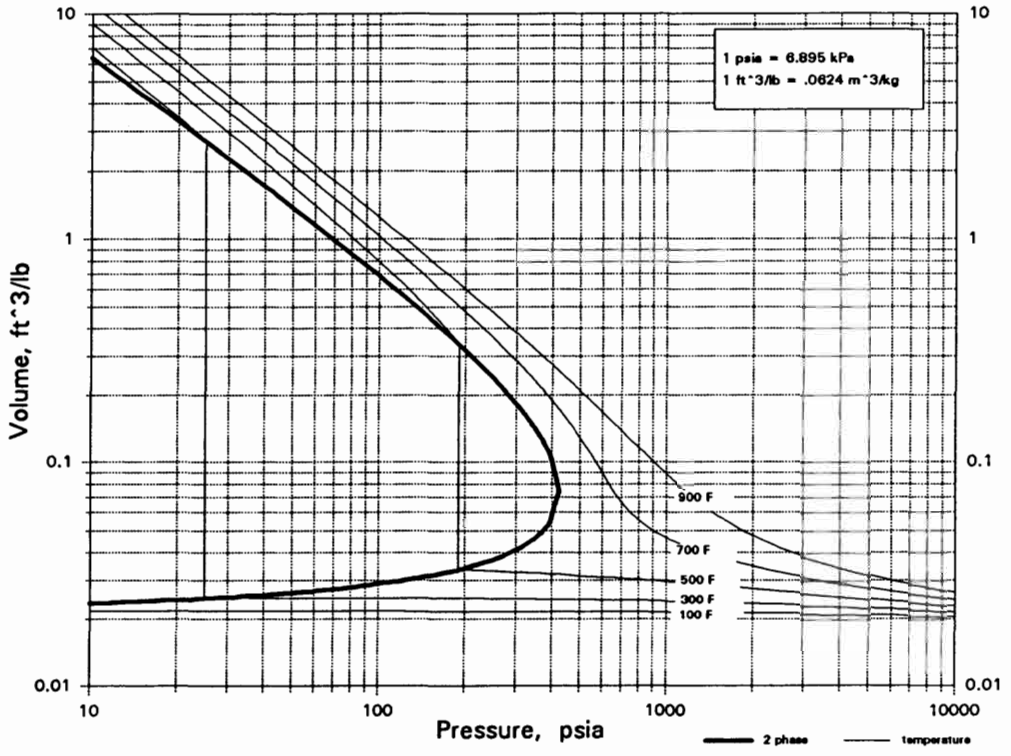


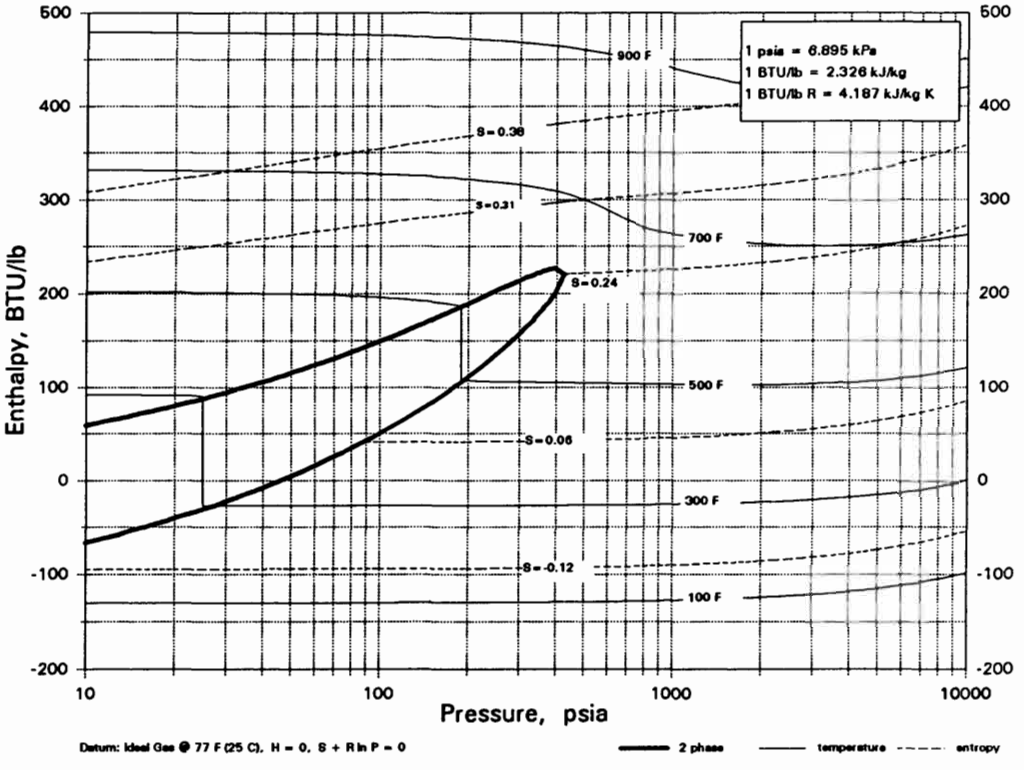
C8H16	cis-1-2-DIMETHYLCYCLOHEXANE



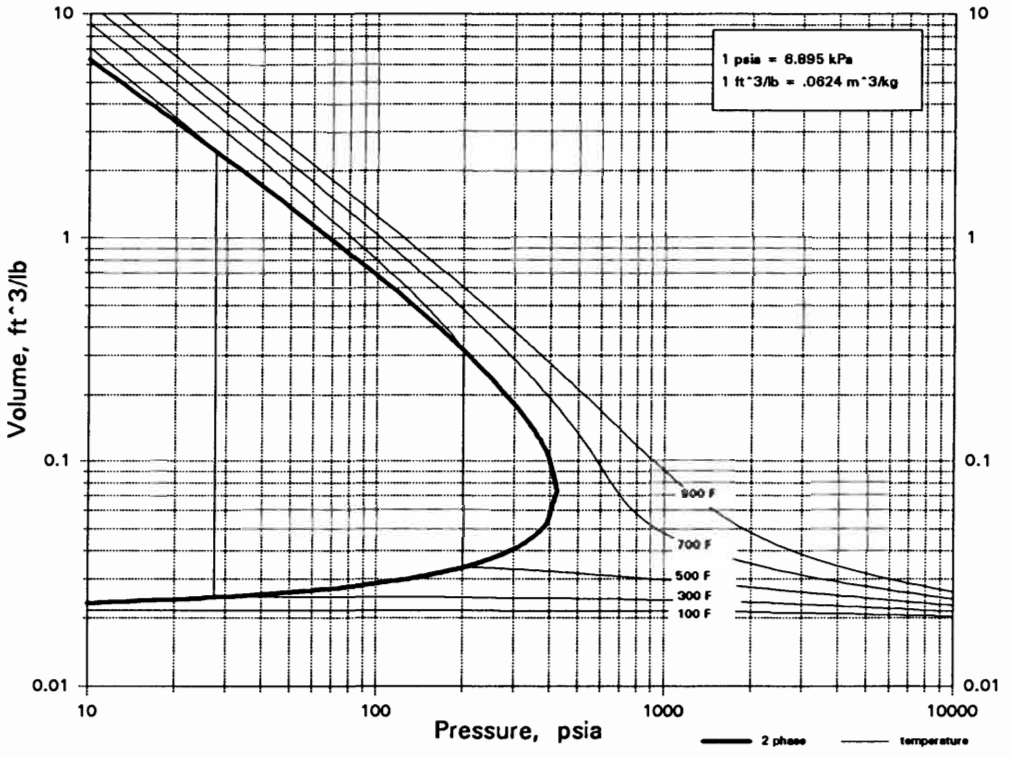


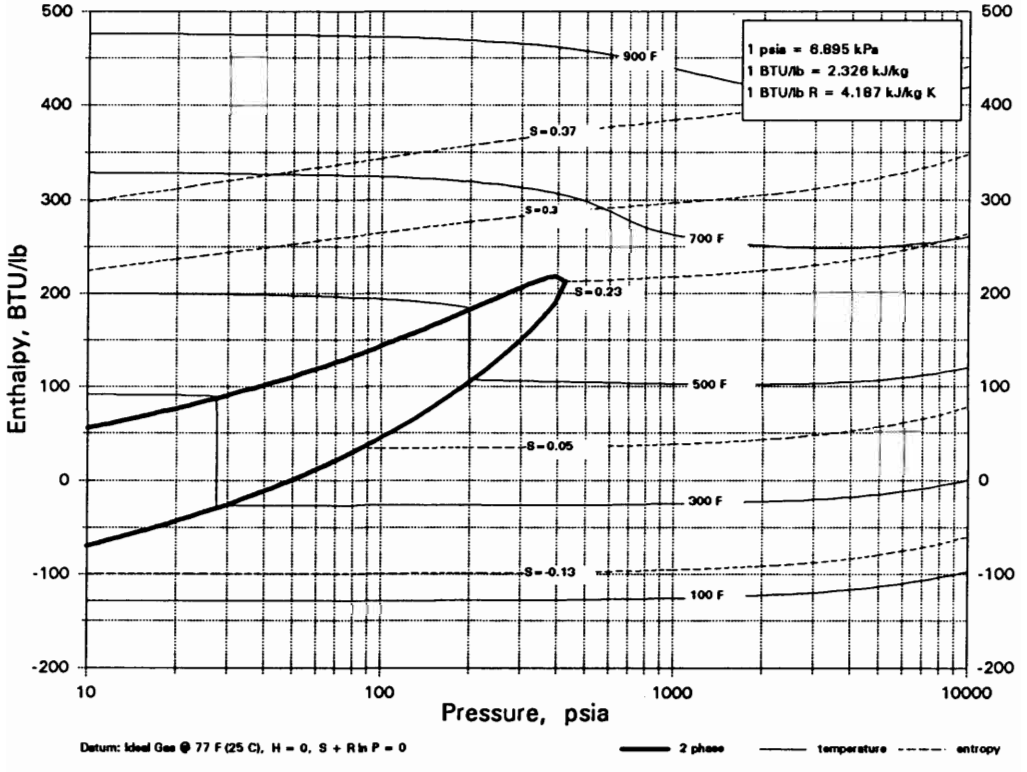
C8H16 trans-1-2-DIMETHYLCYCLOHEXANE





C8H16 cis-1-3-DIMETHYLCYCLOHEXANE





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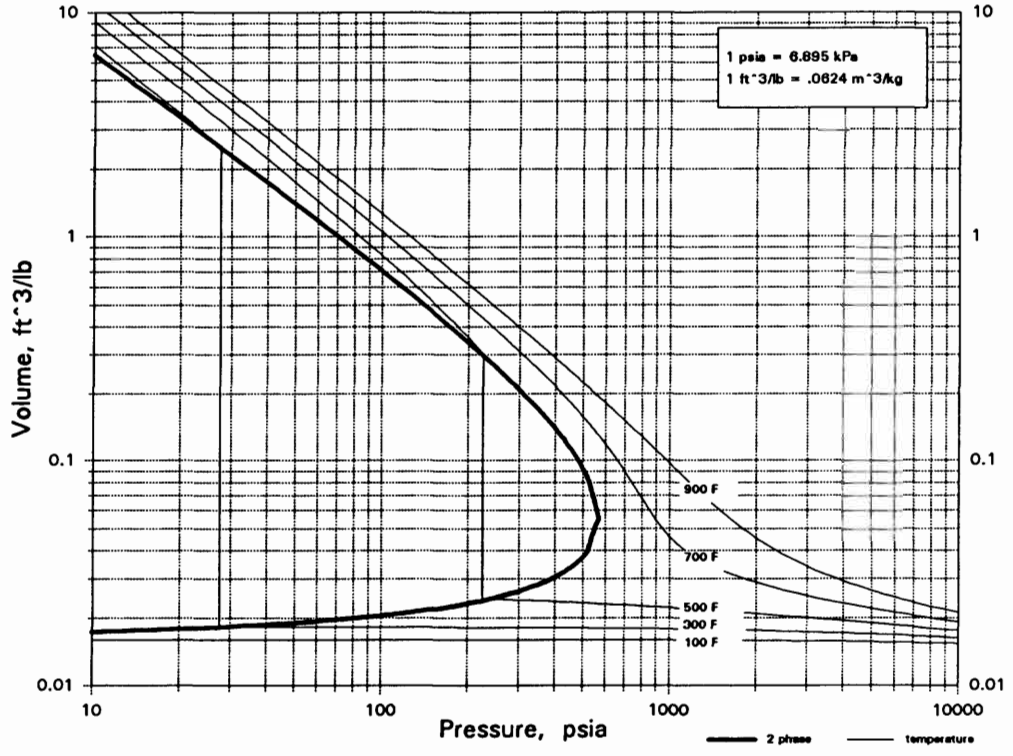
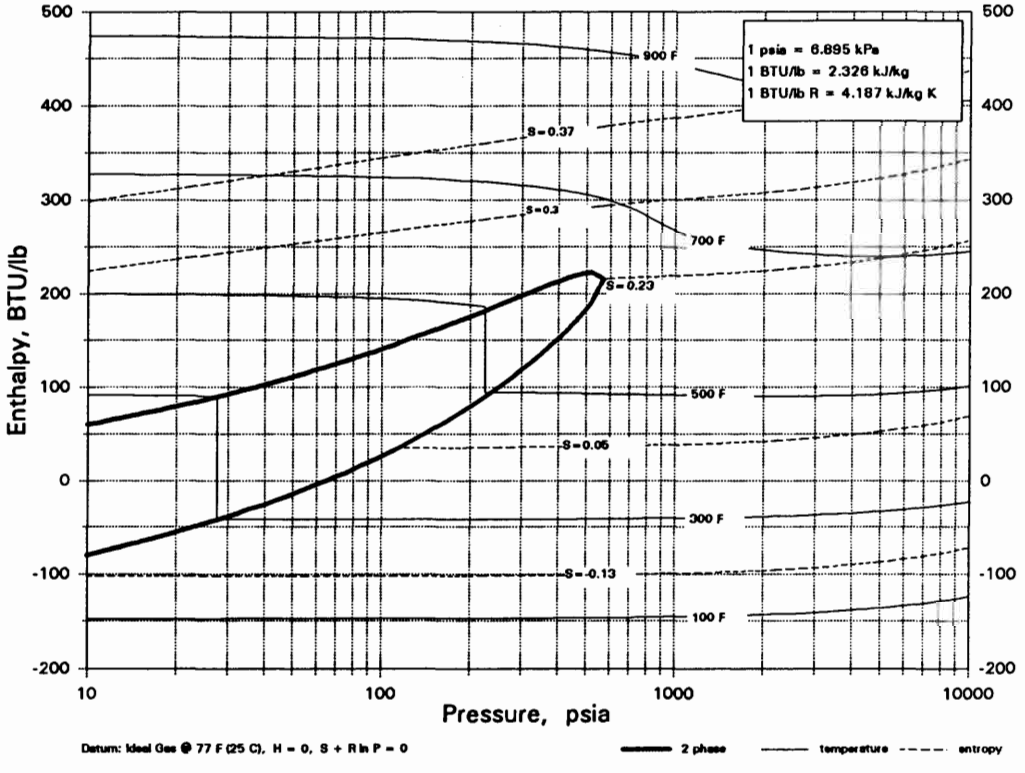
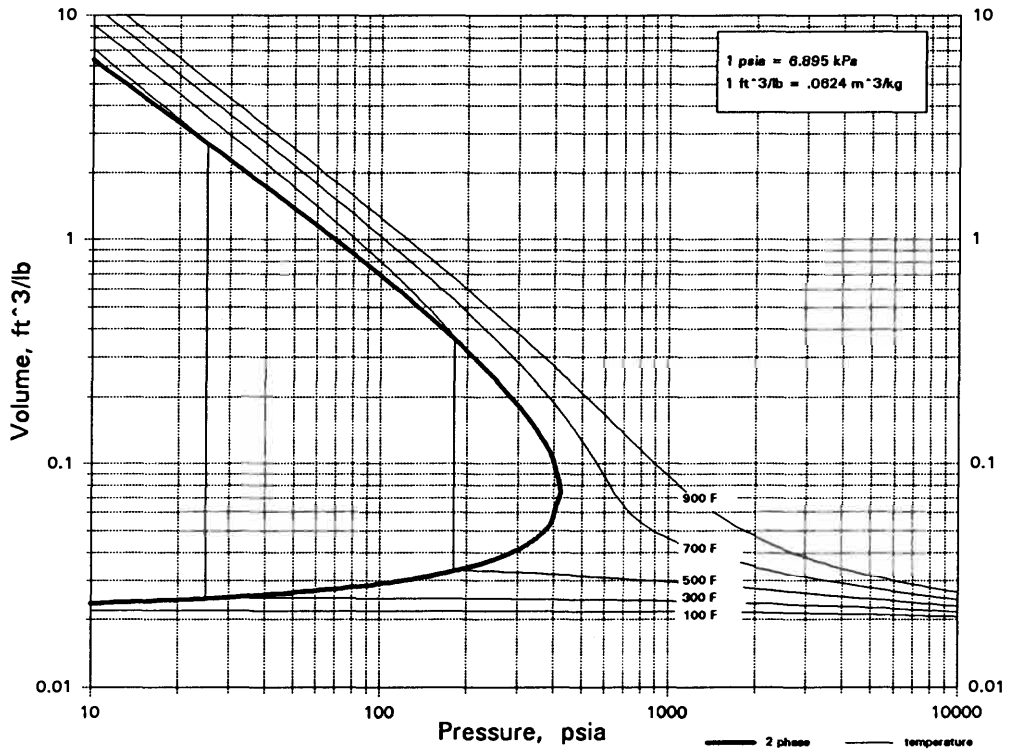
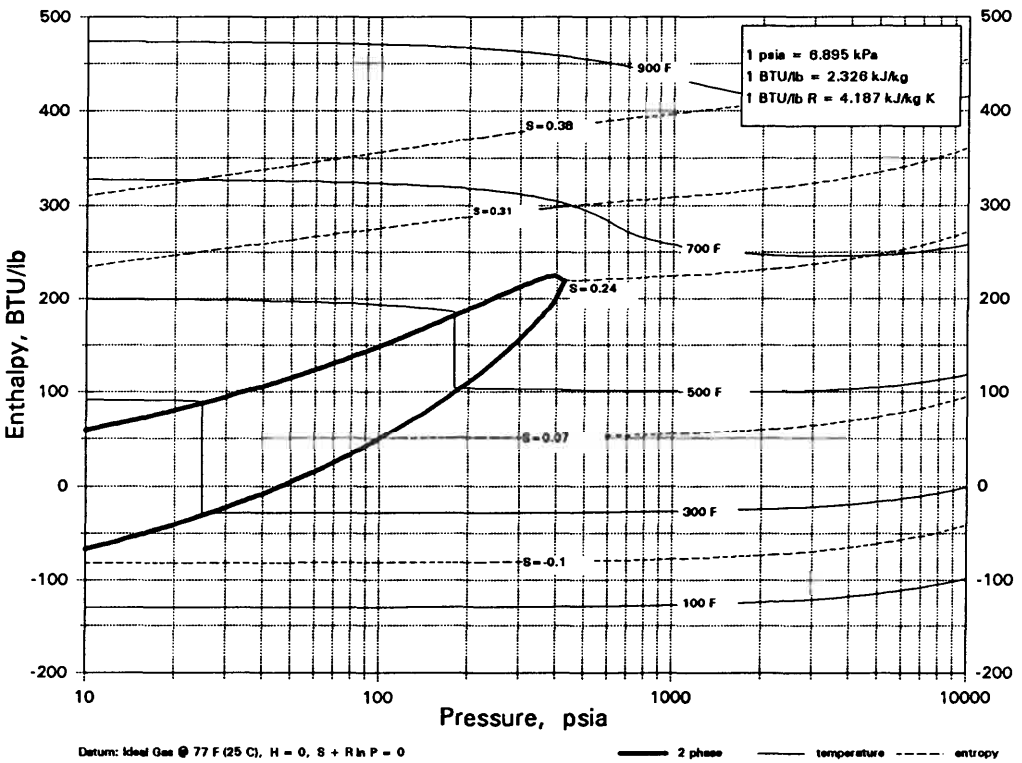


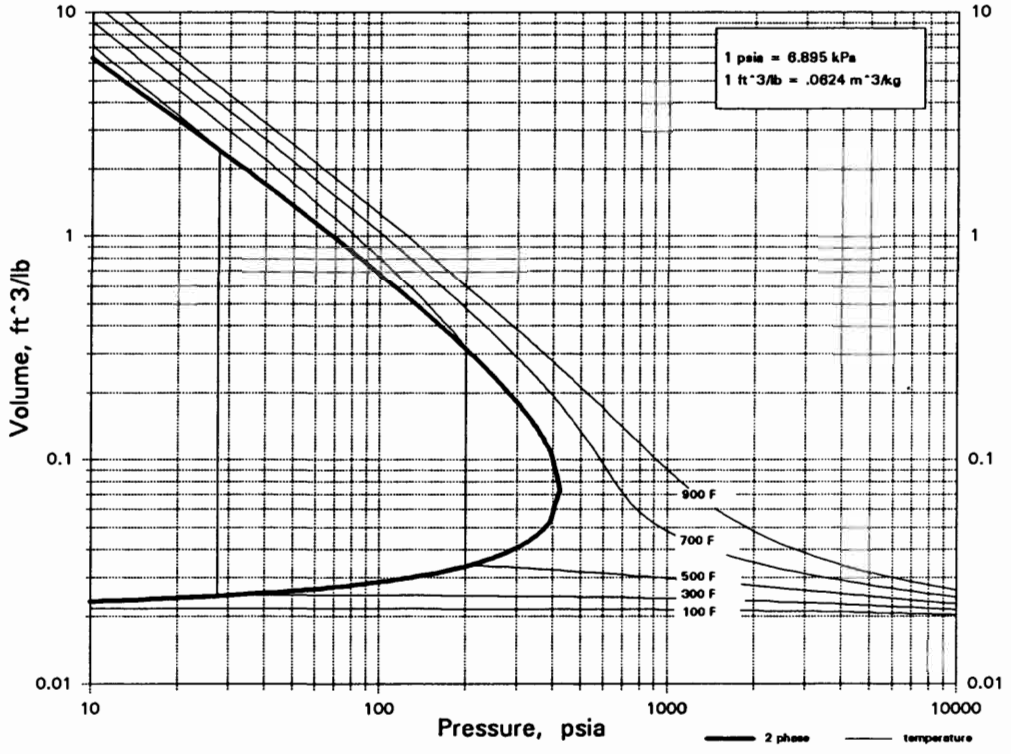


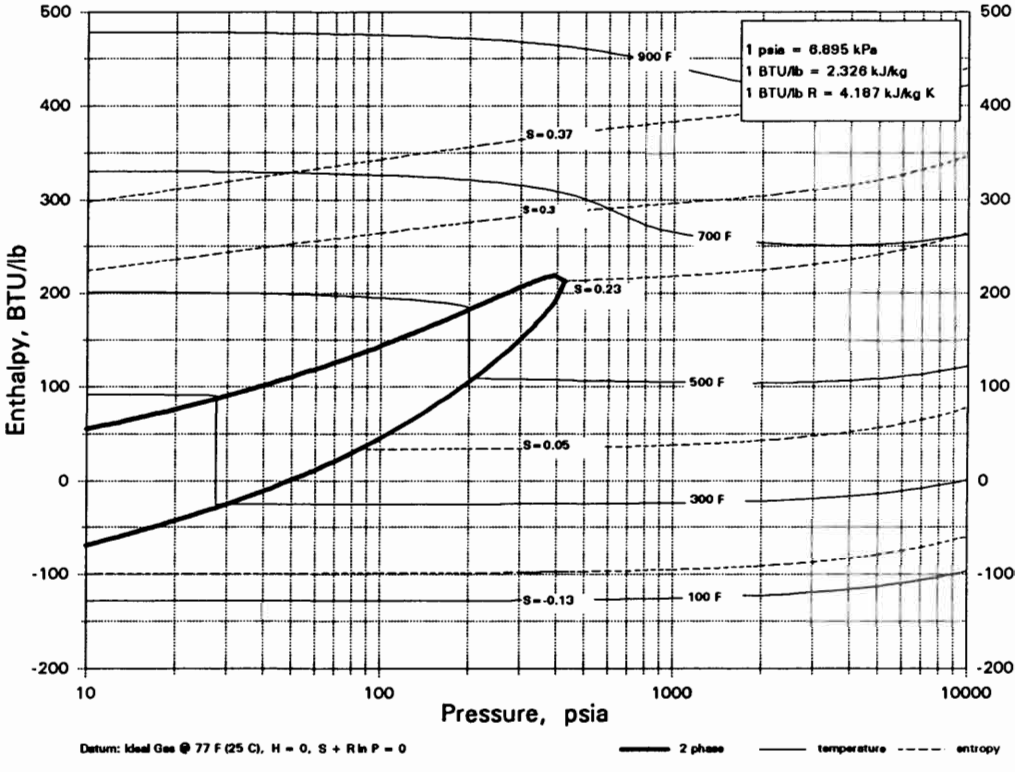
C8H16 cis-1-4-DIMETHYLCYCLOHEXANE



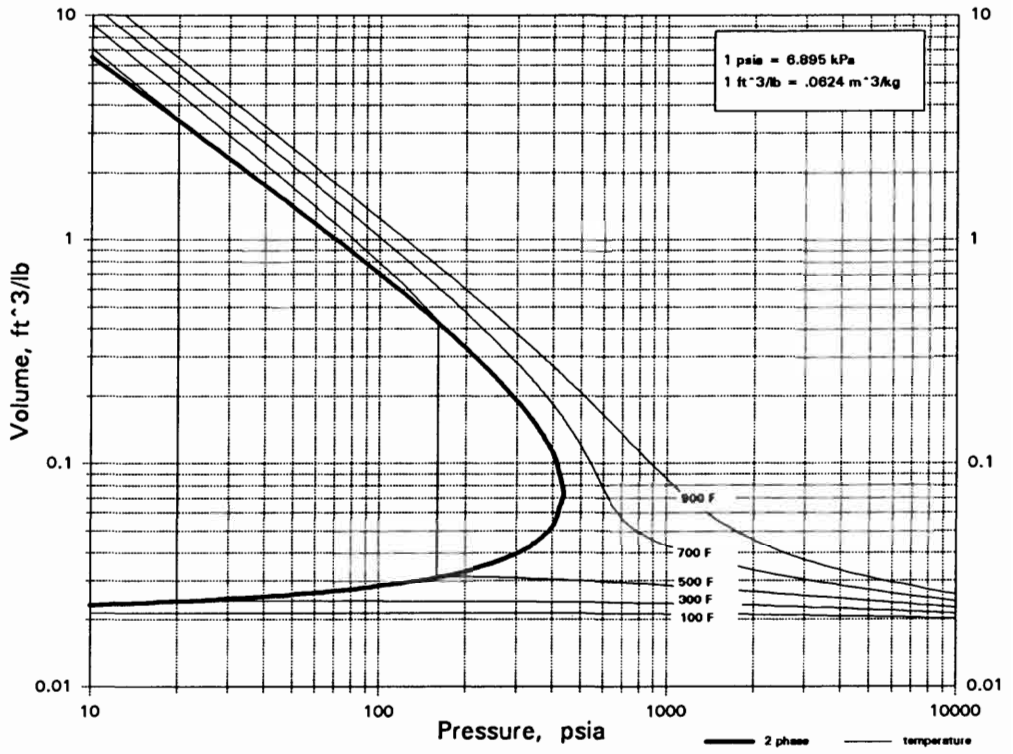


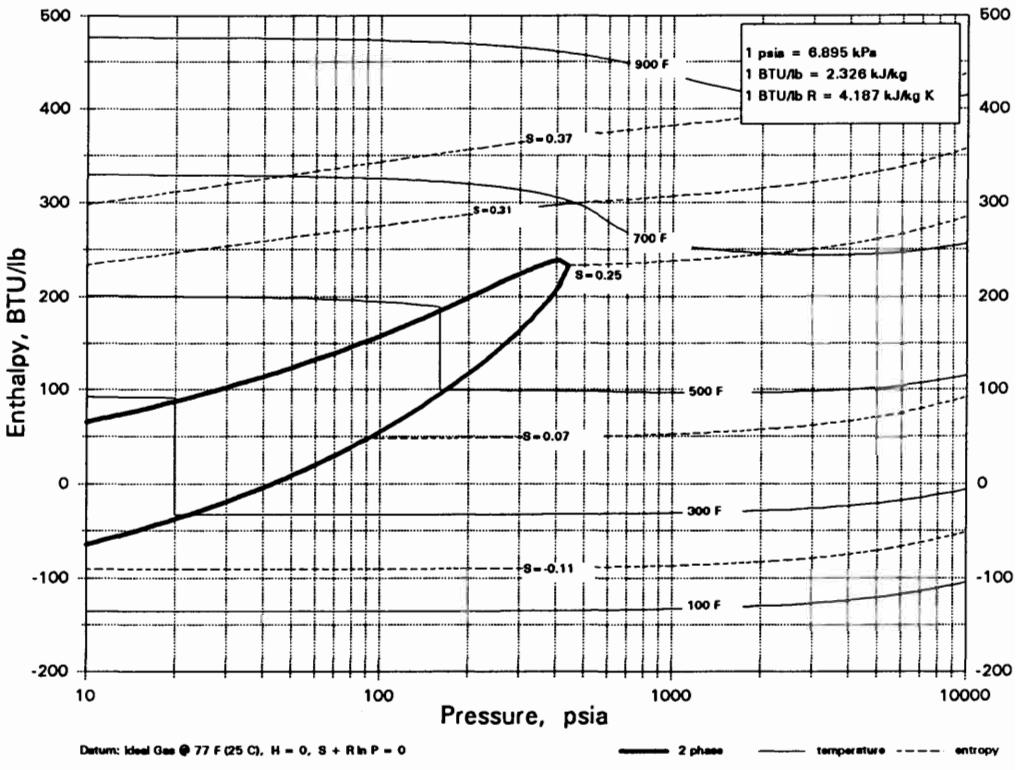
C8H16 trans-1-4-DIMETHYLCYCLOHEXANE



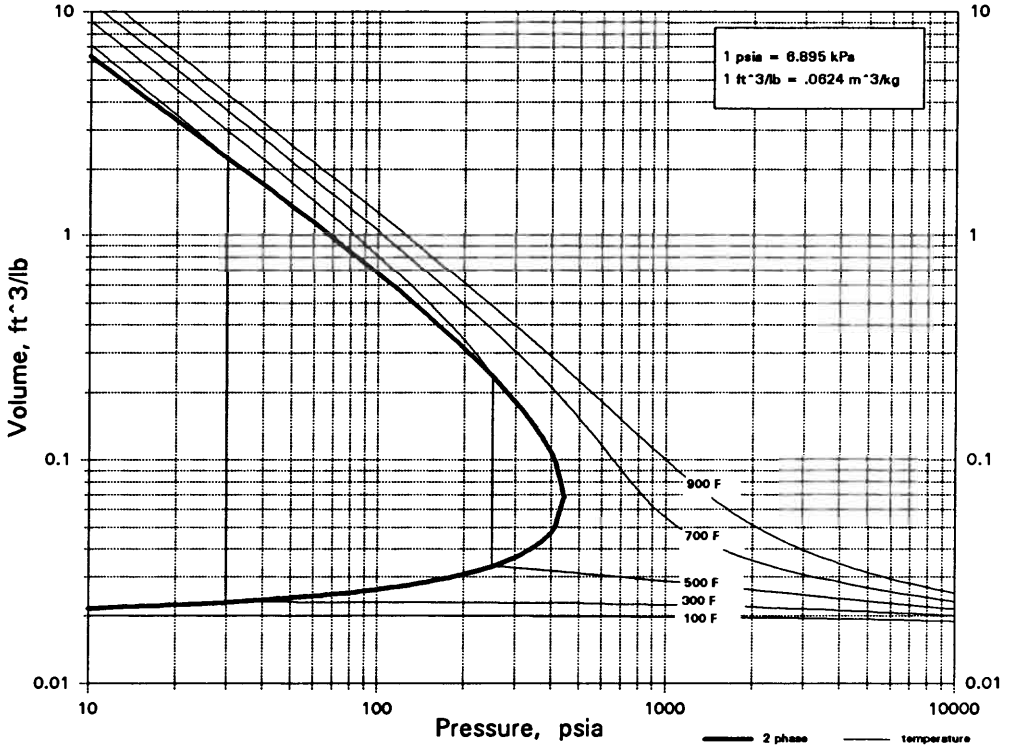


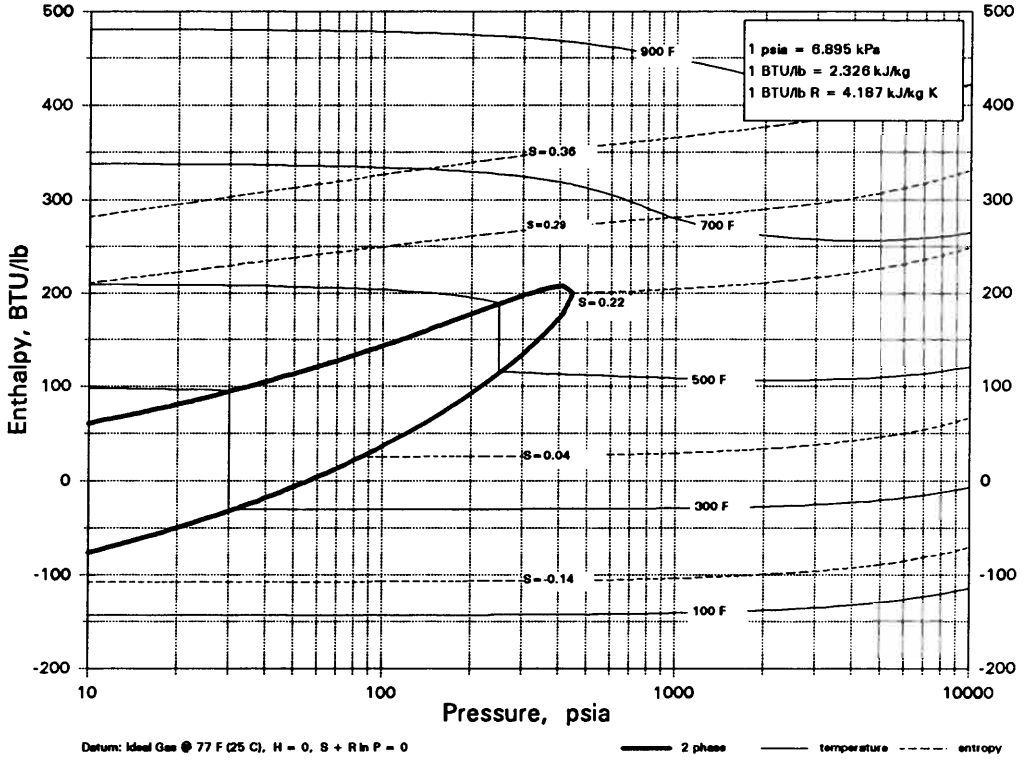
C8H16 ETHYLCYCLOHEXANE



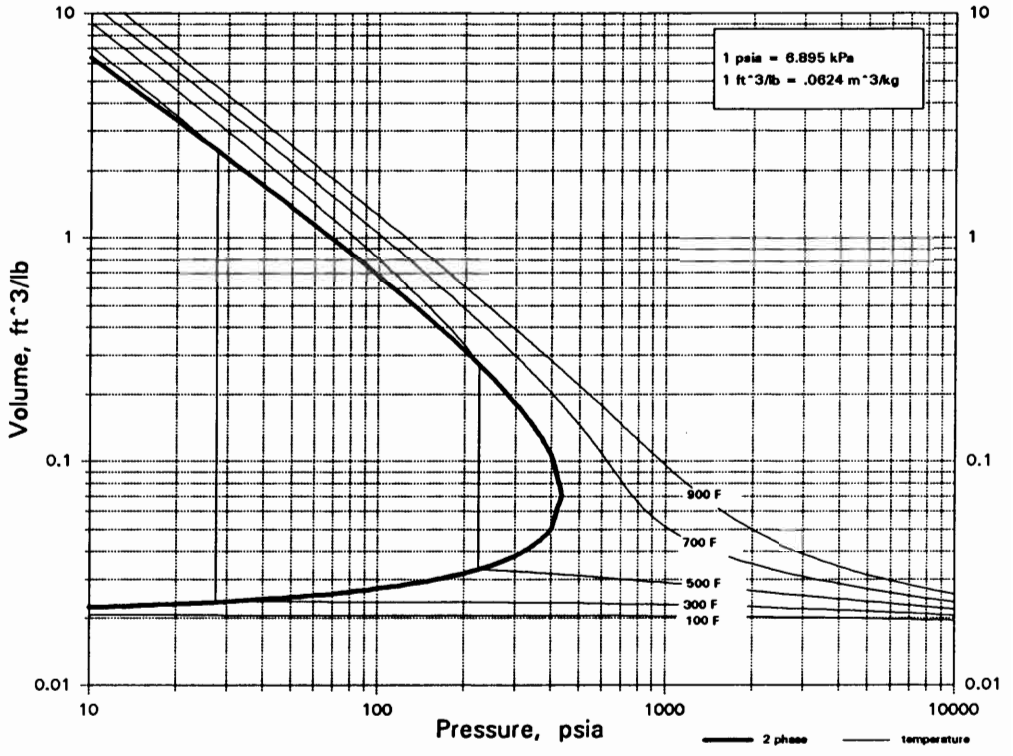


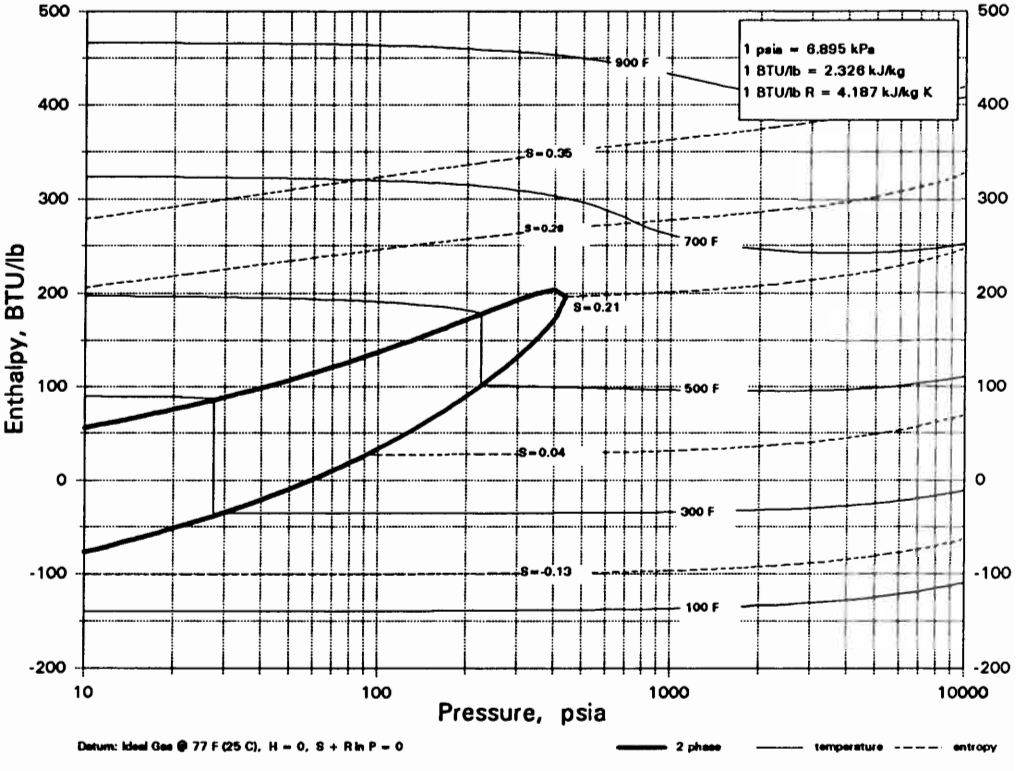
C8H16	2-ETHYL-1-HEXENE



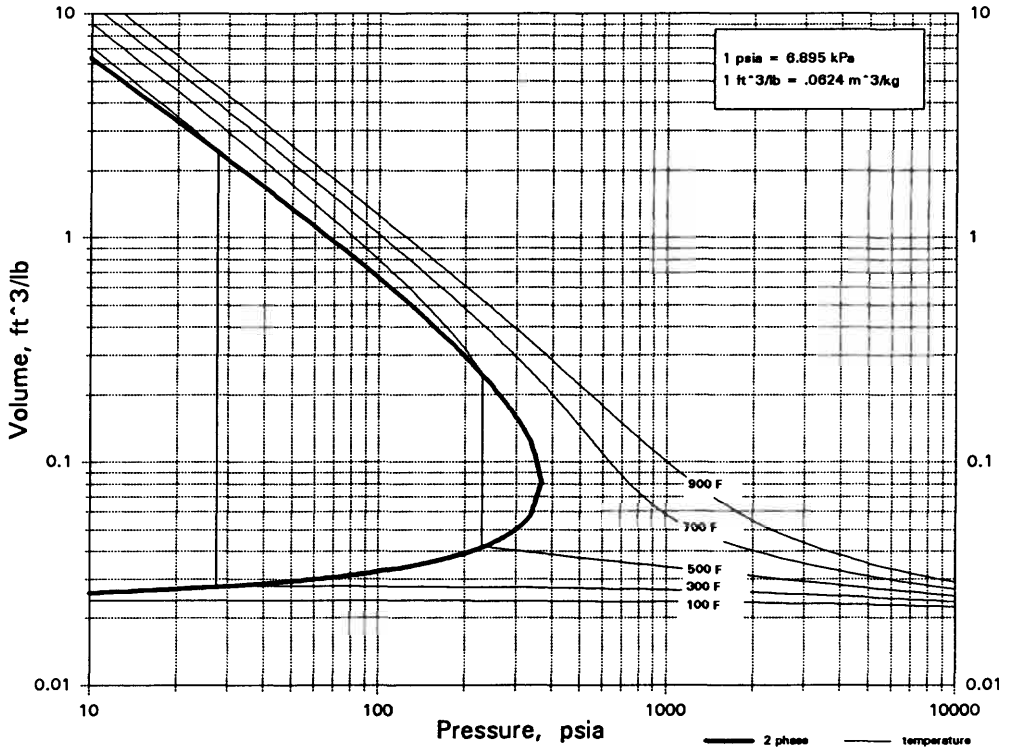


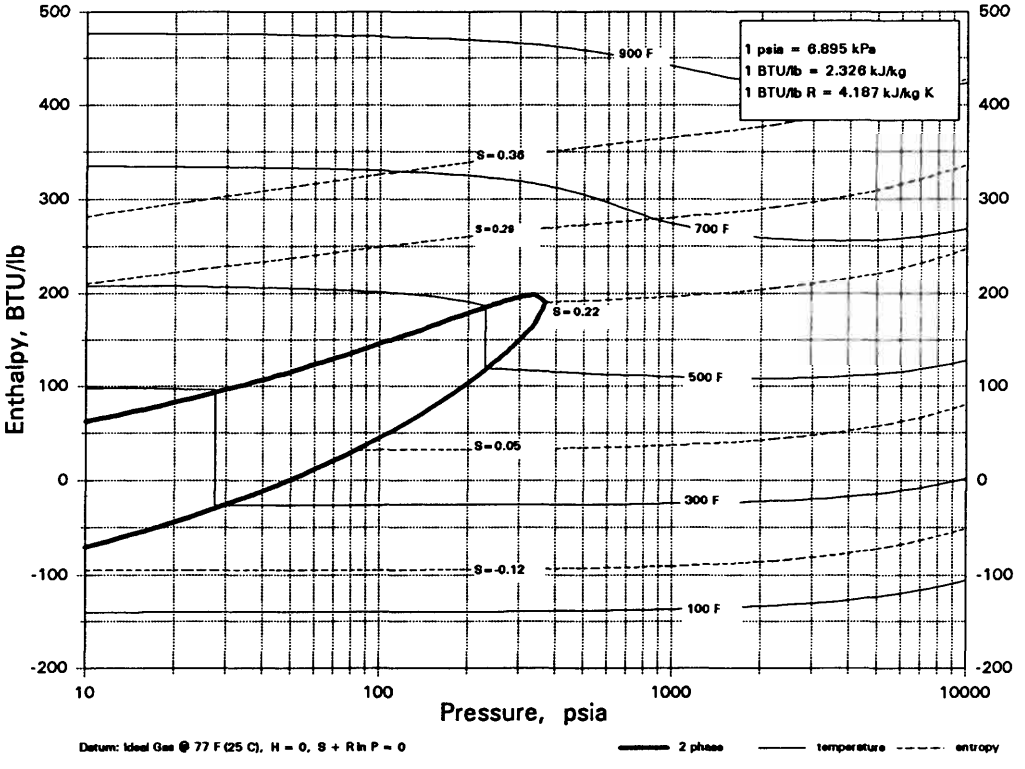
C8H16 1-METHYL-1-ETHYLCYCLOPENTANE



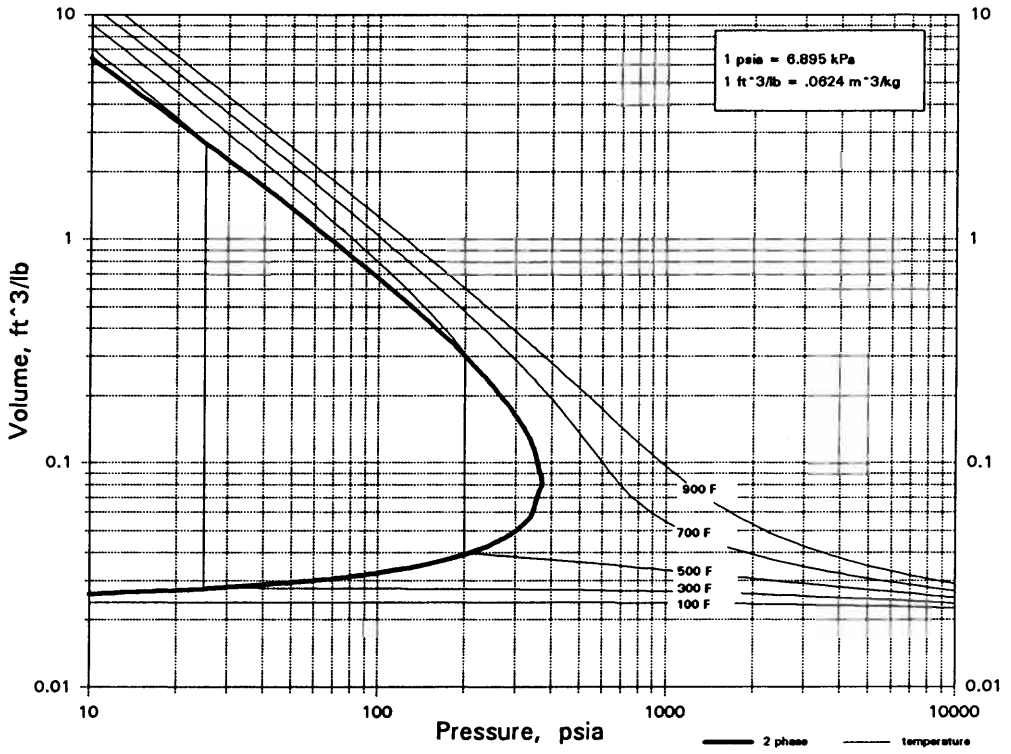


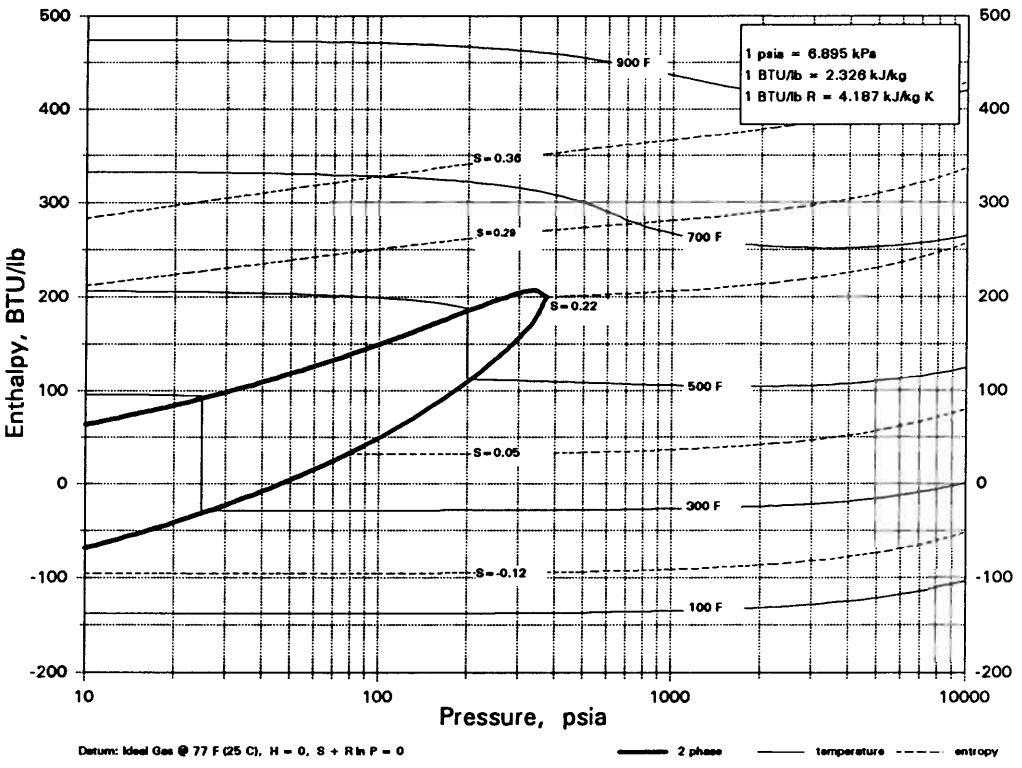
C8H16 1-OCTENE



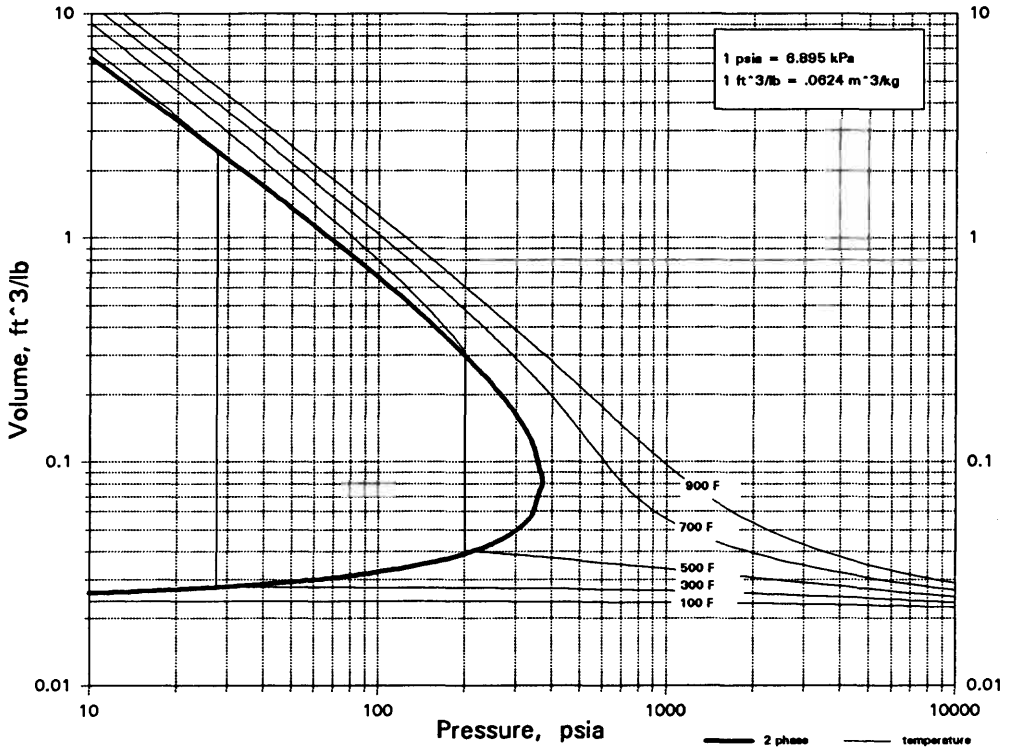


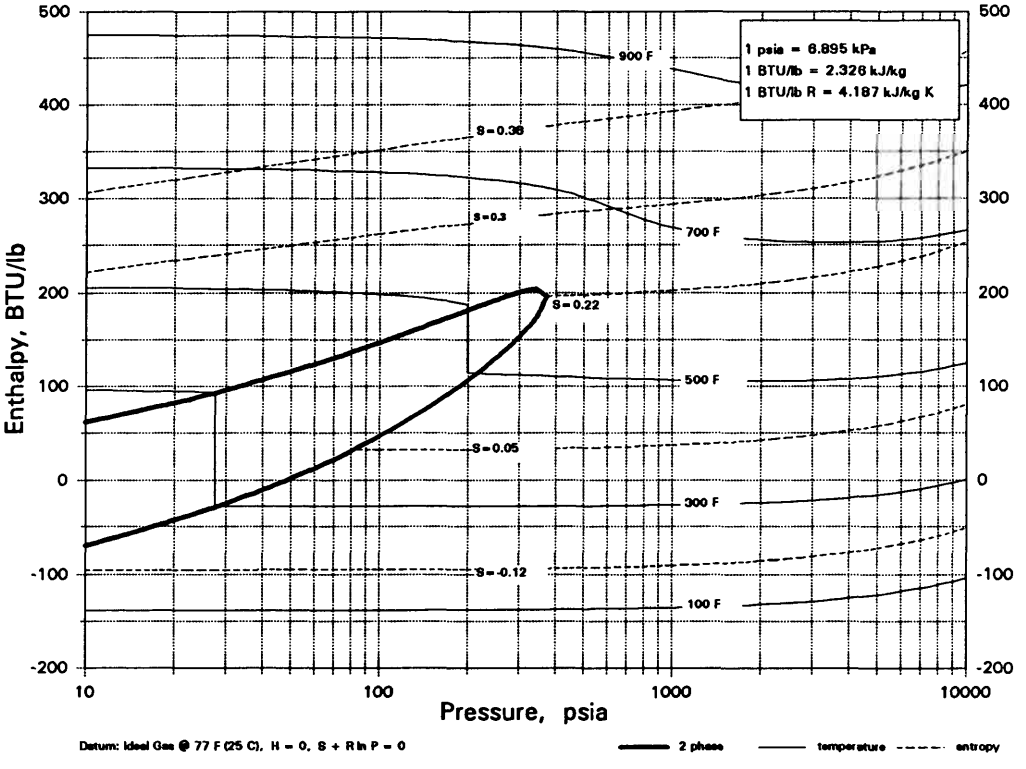
C8H16 trans-2-OCTENE



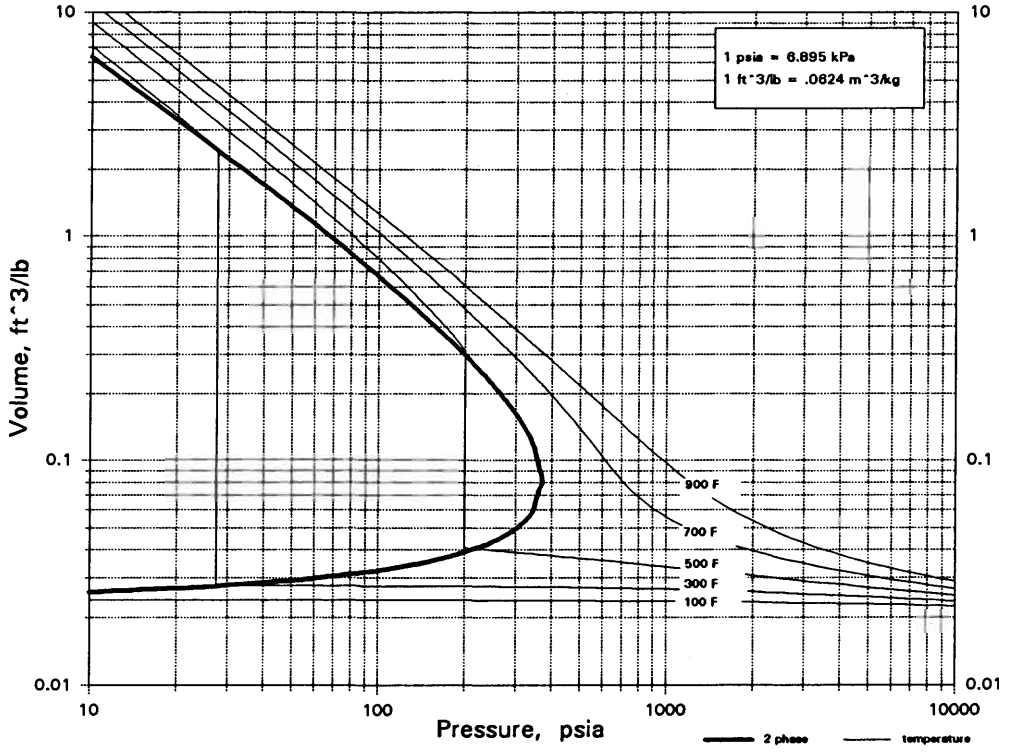


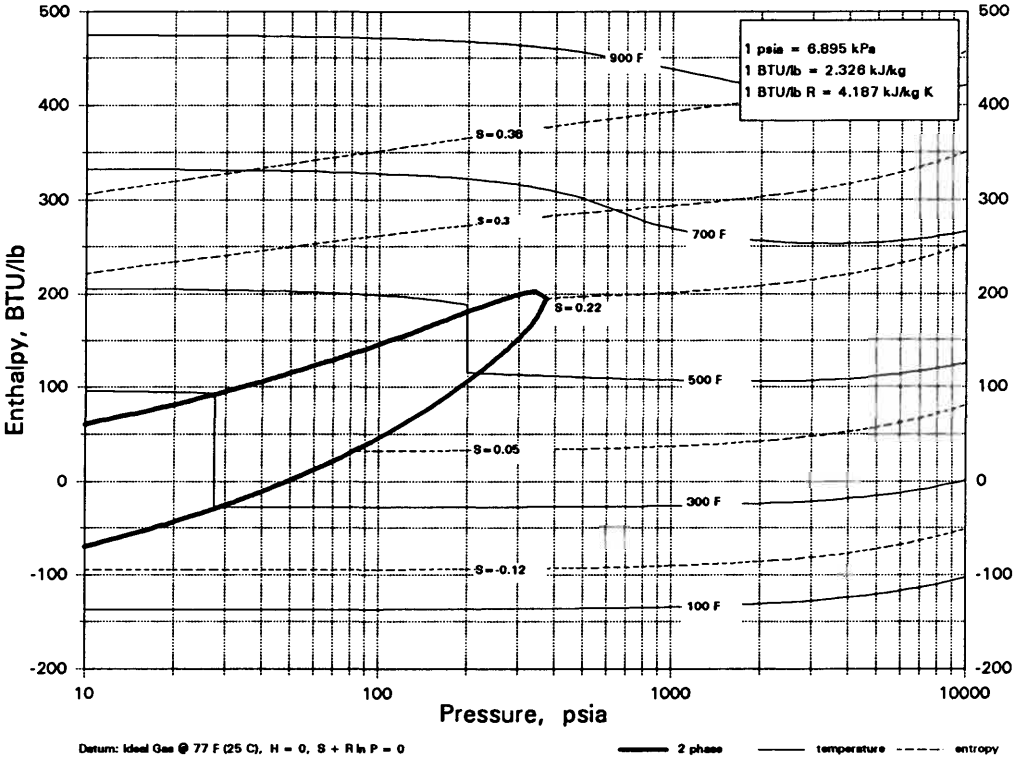
C8H16 trans-3-OCTENE



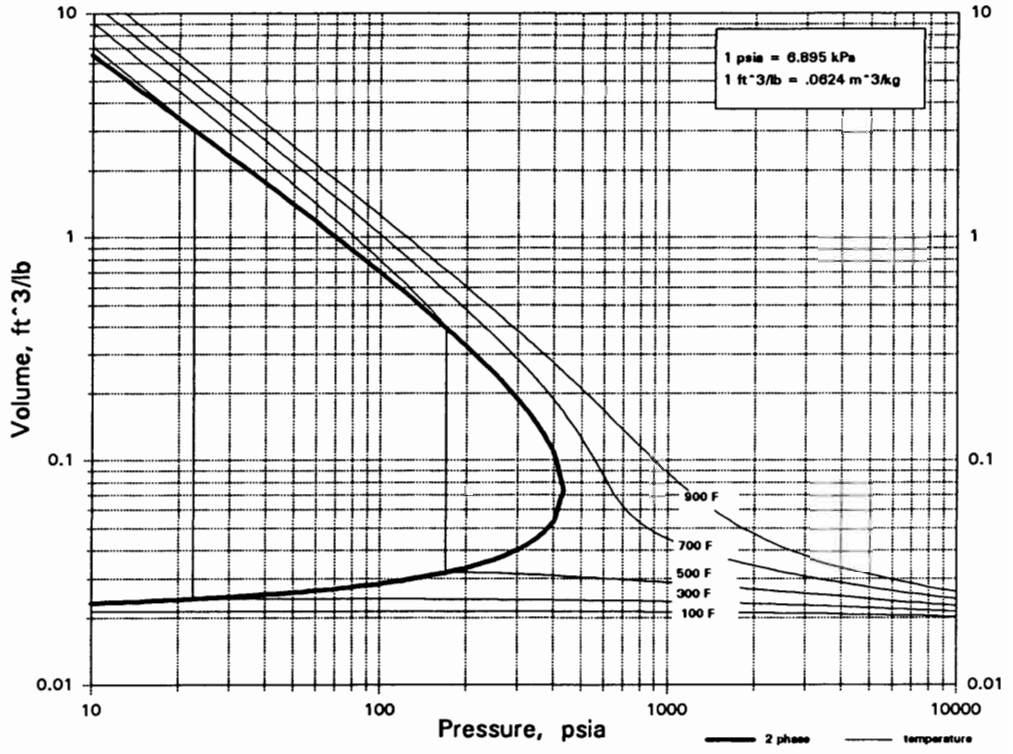


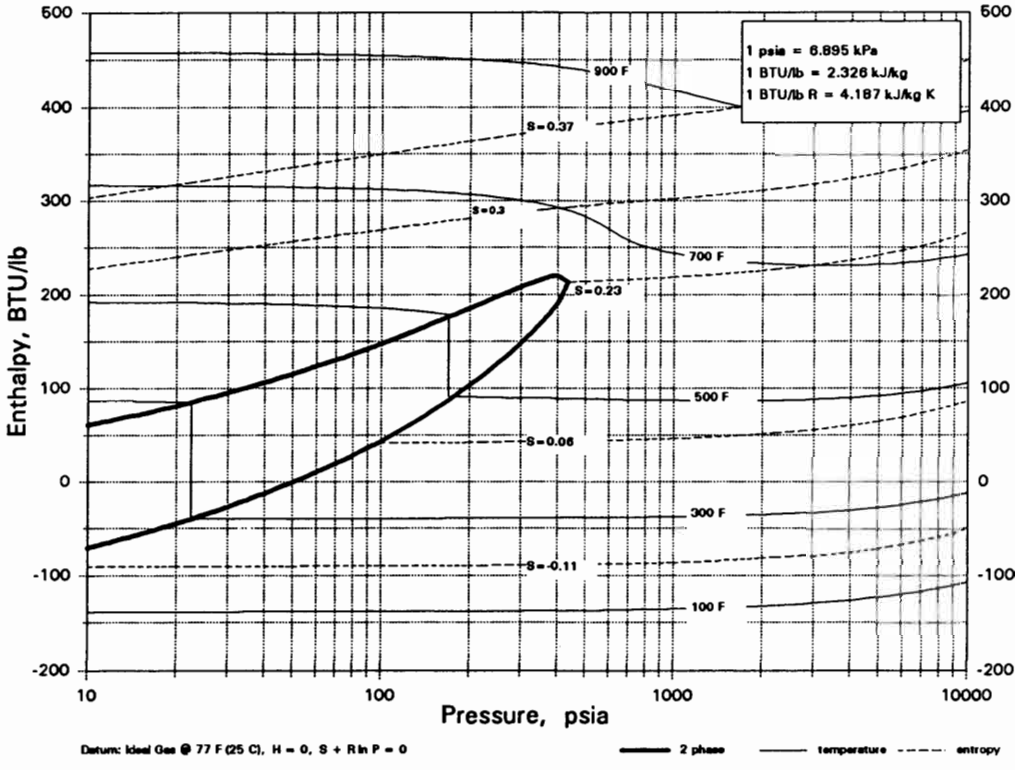
C8H16 trans-4-OCTENE



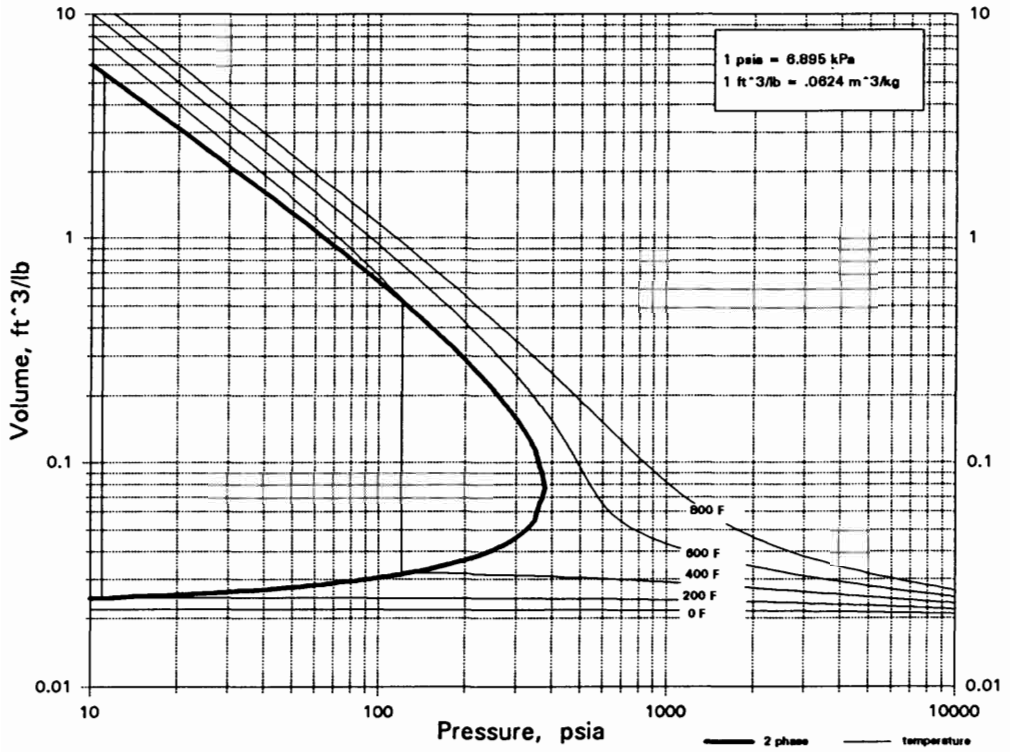


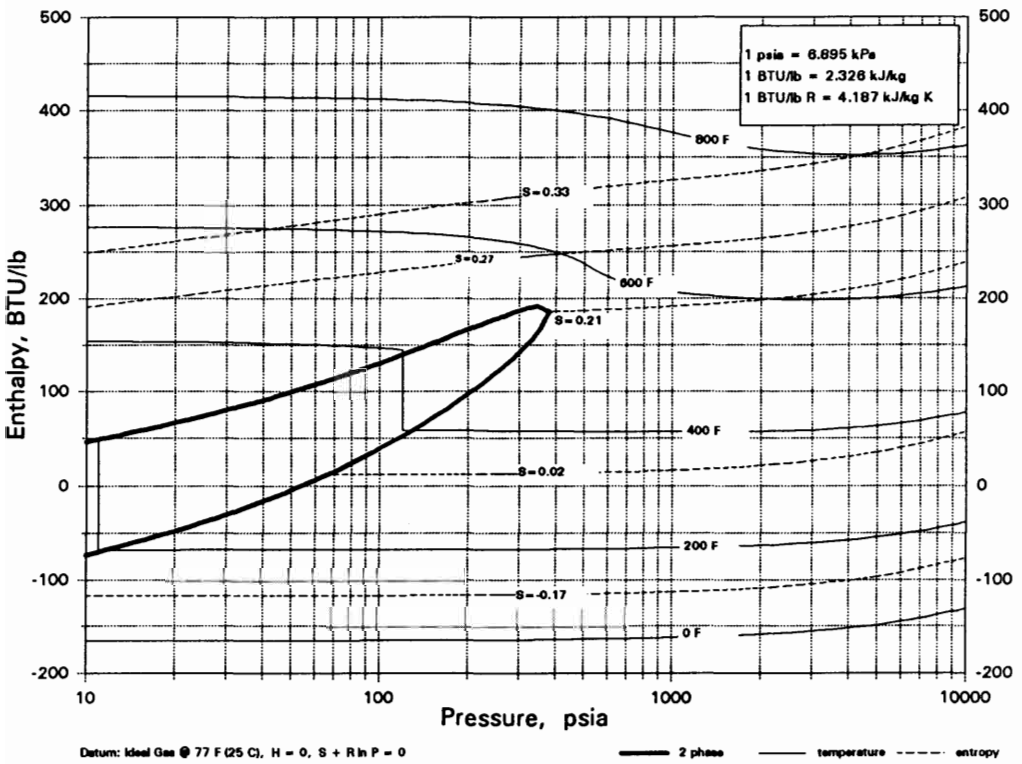
C8H16 n-PROPYLCYCLOPENTANE



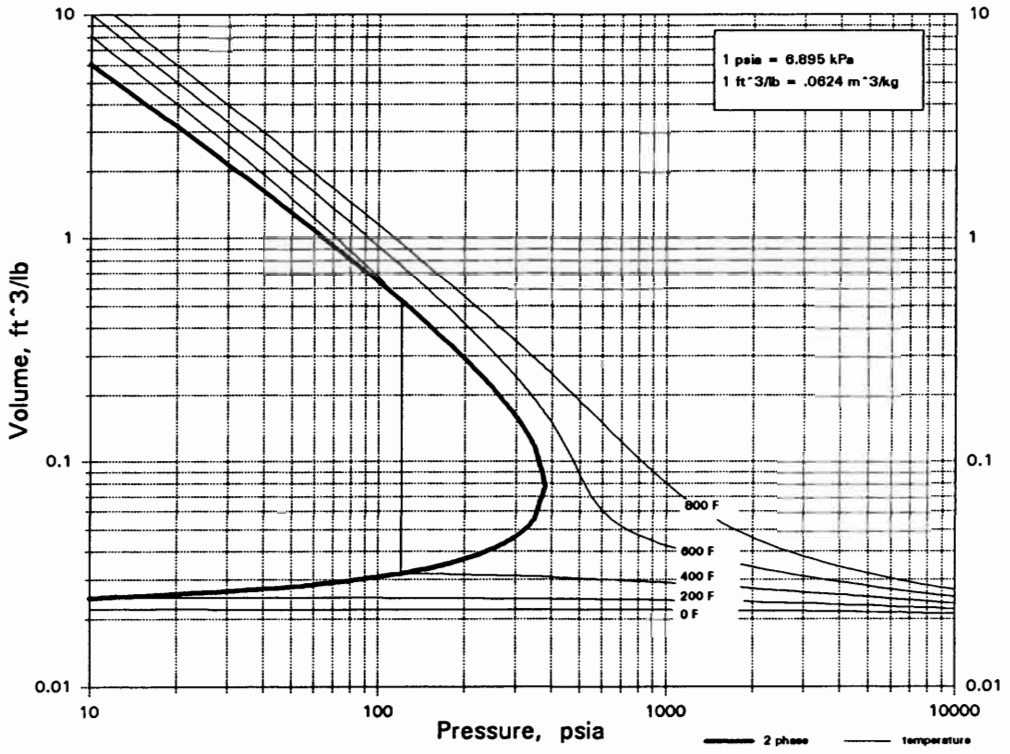


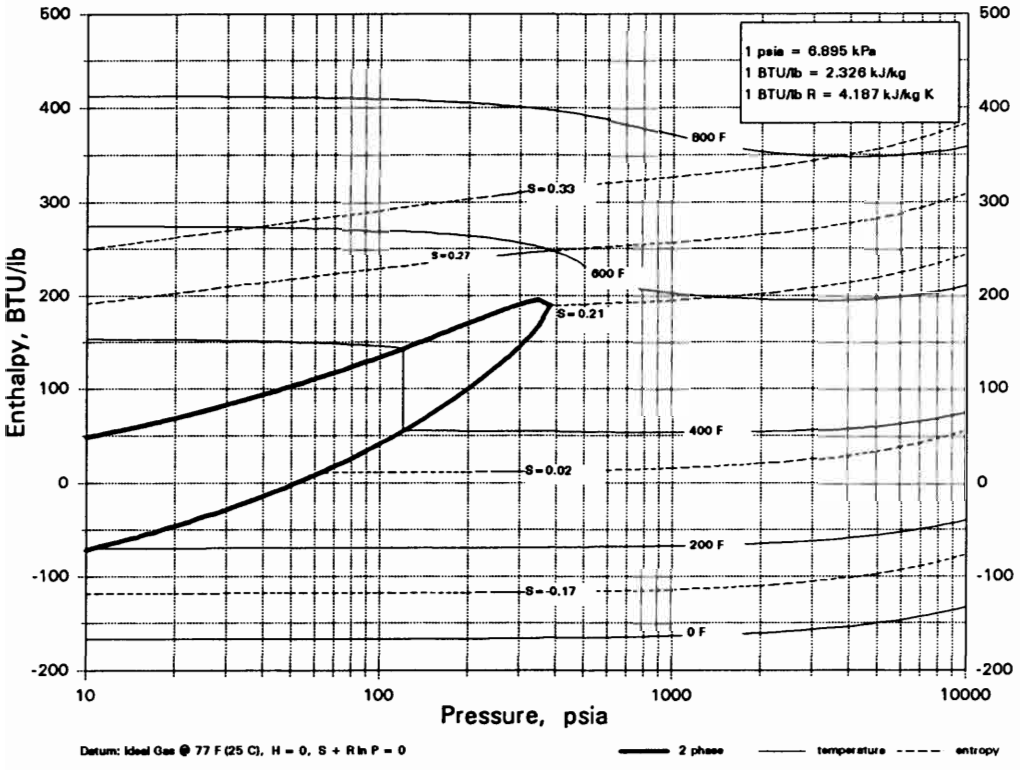
C8H16 2-4-4-TRIMETHYL-1-PENTENE



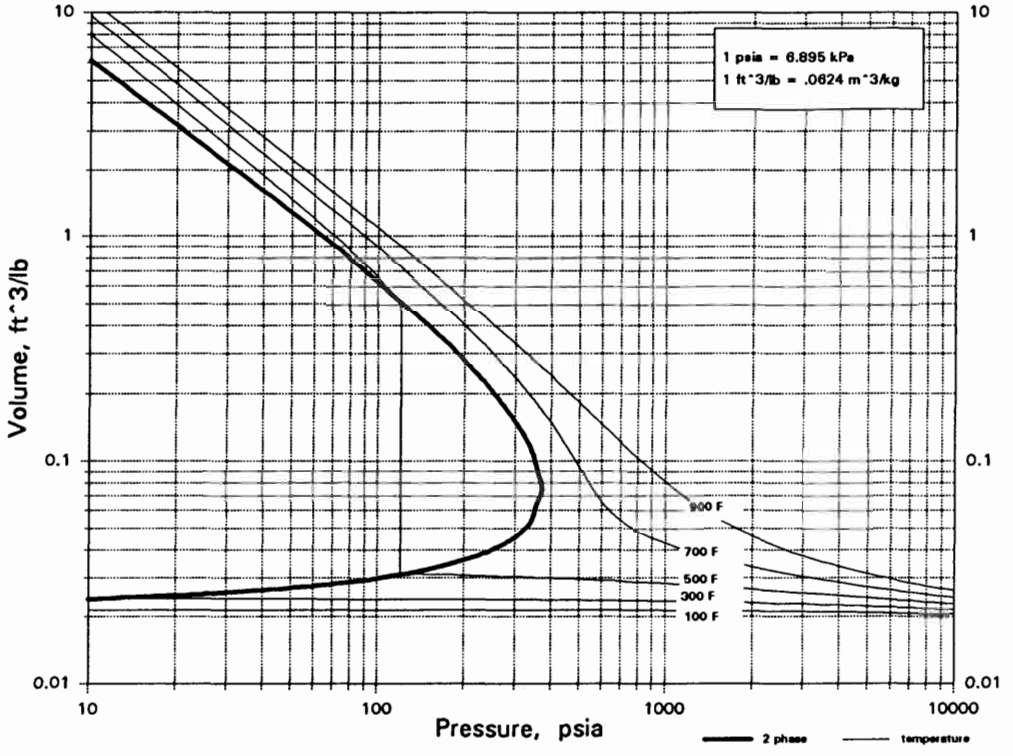


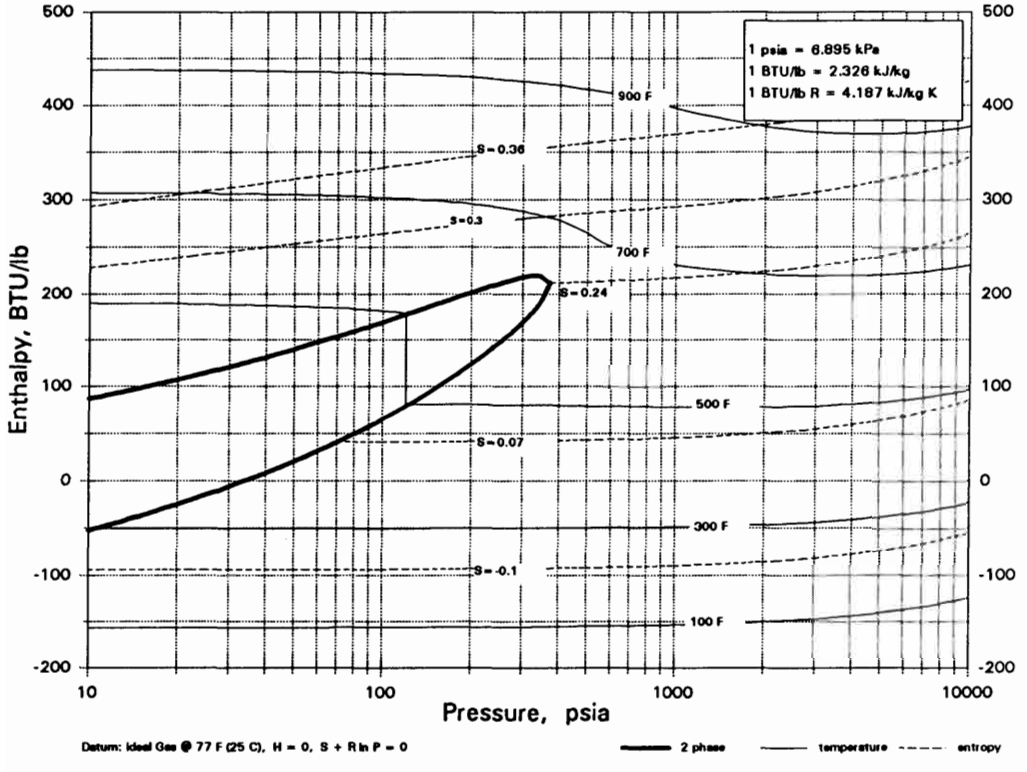
C8H16 2-4-4-TRIMETHYL-2-PENTENE



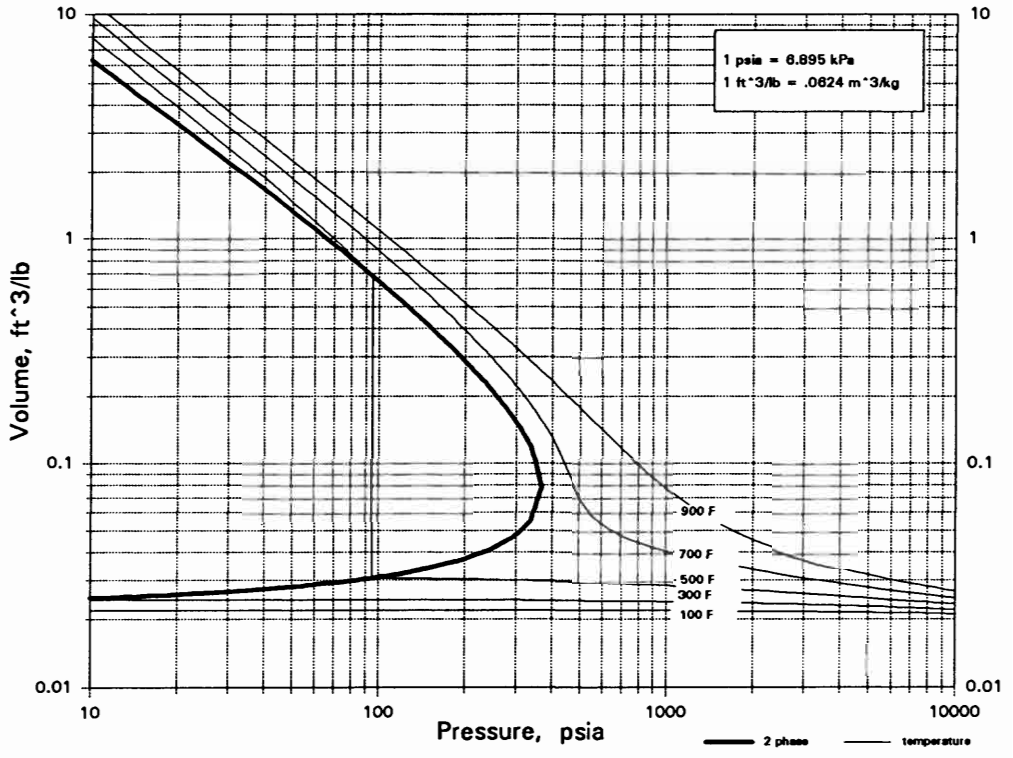


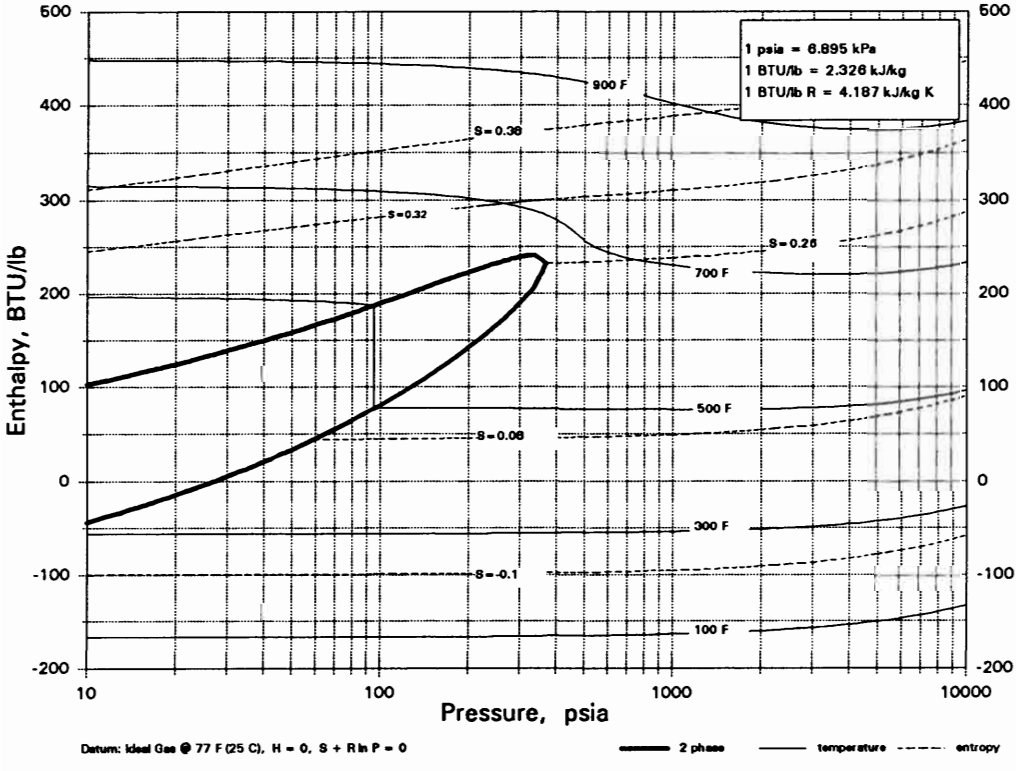
C8H16O 2-ETHYLHEXANAL



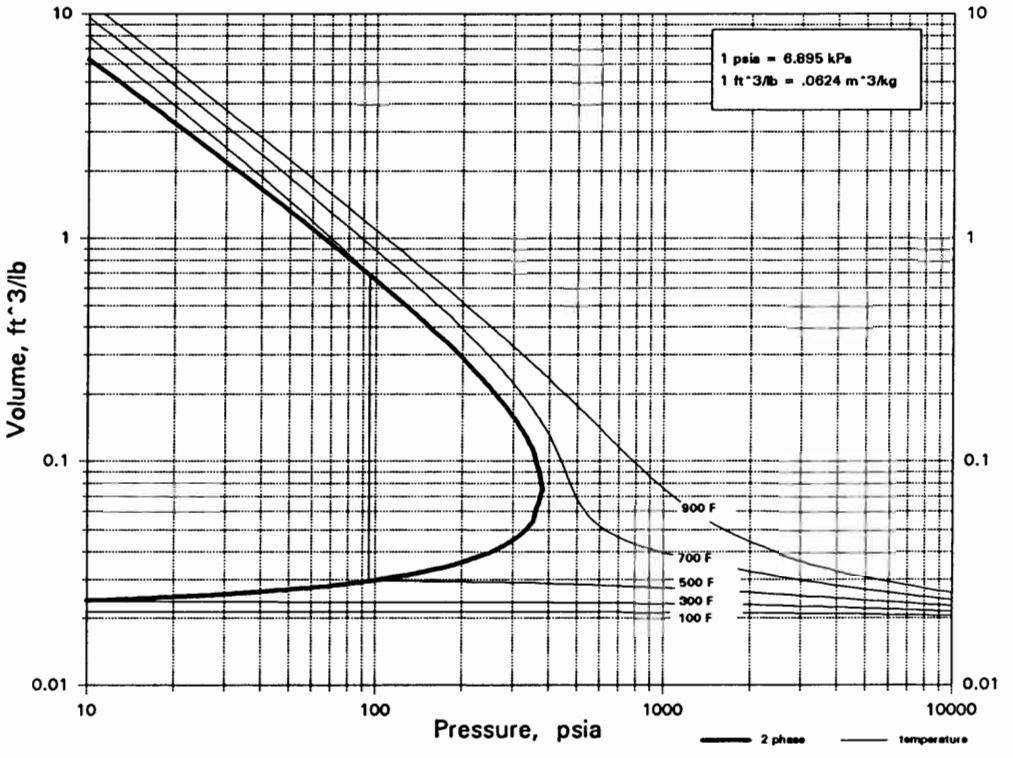


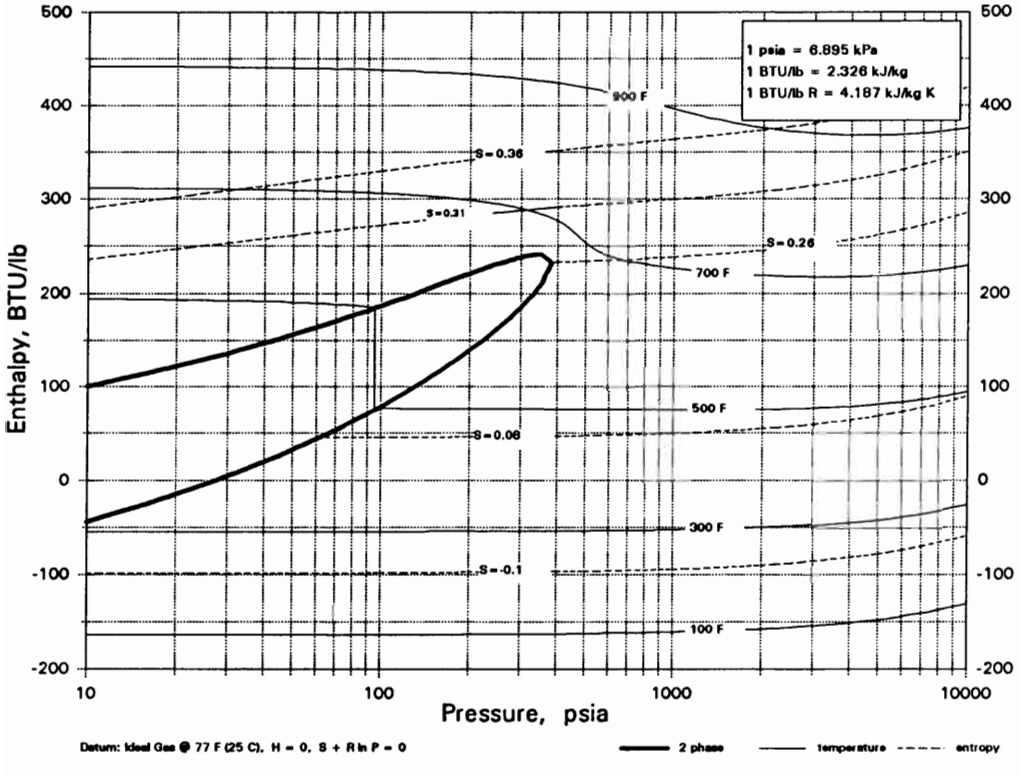
C8H16O 1-OCTANAL



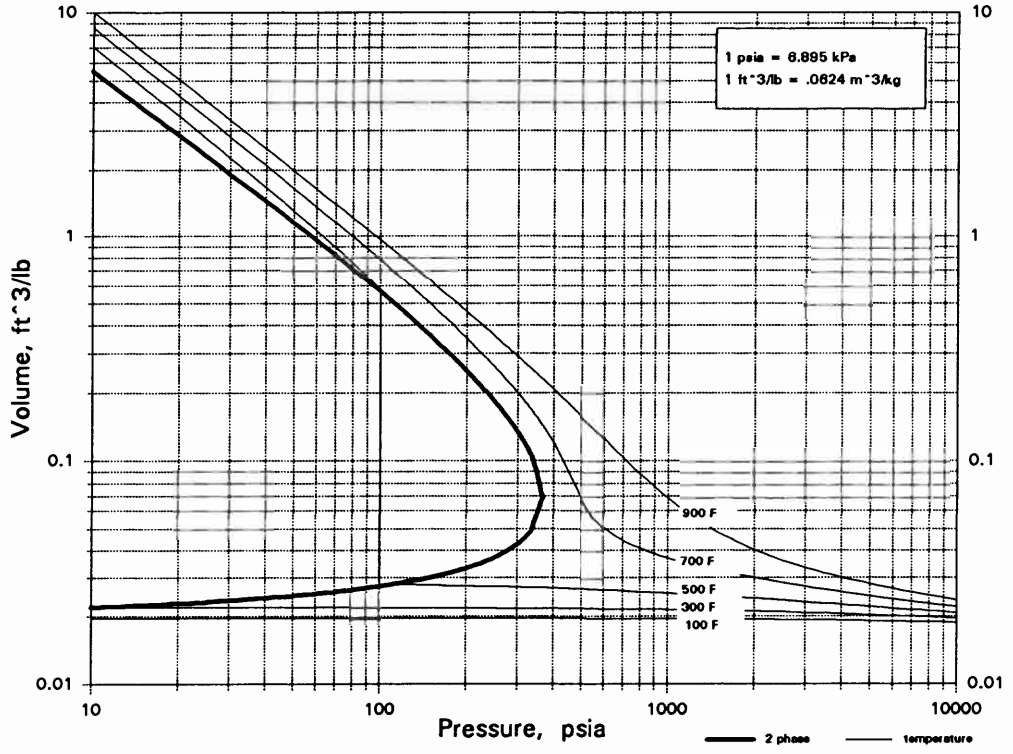


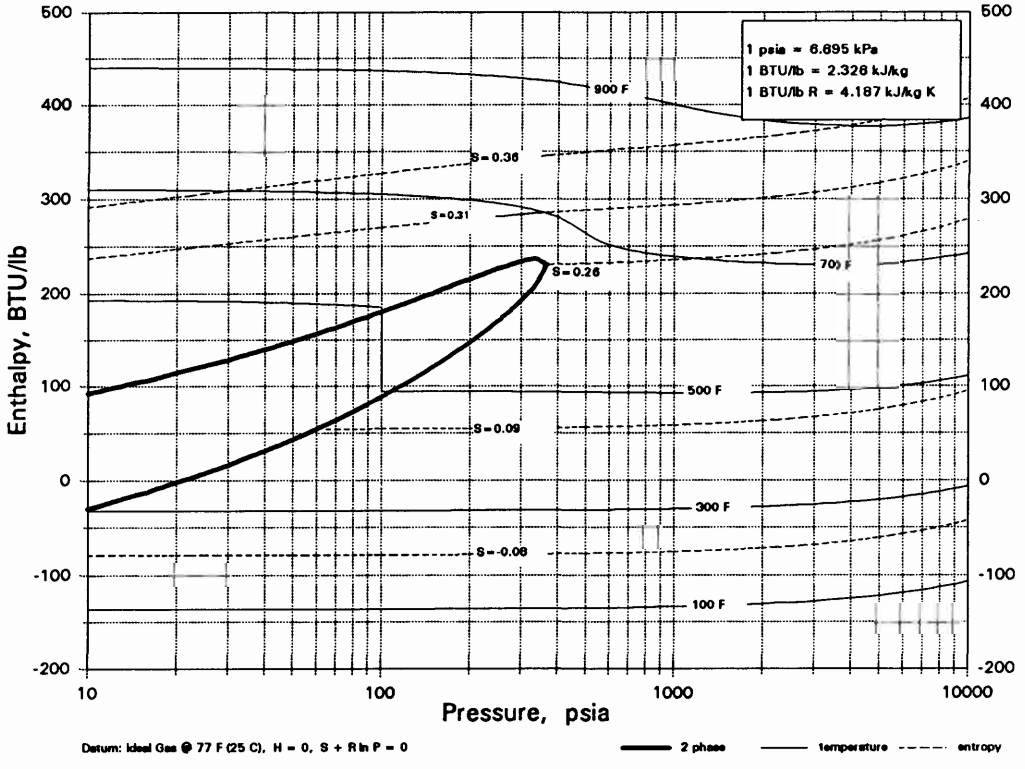
C8H16O 2-OCTANONE



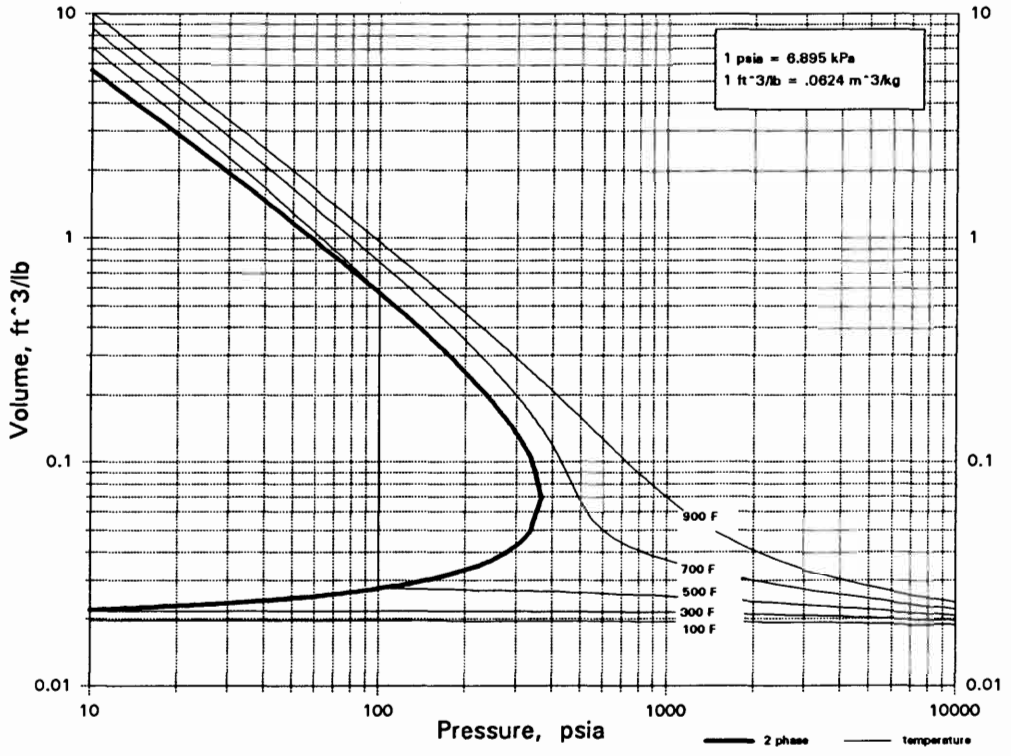


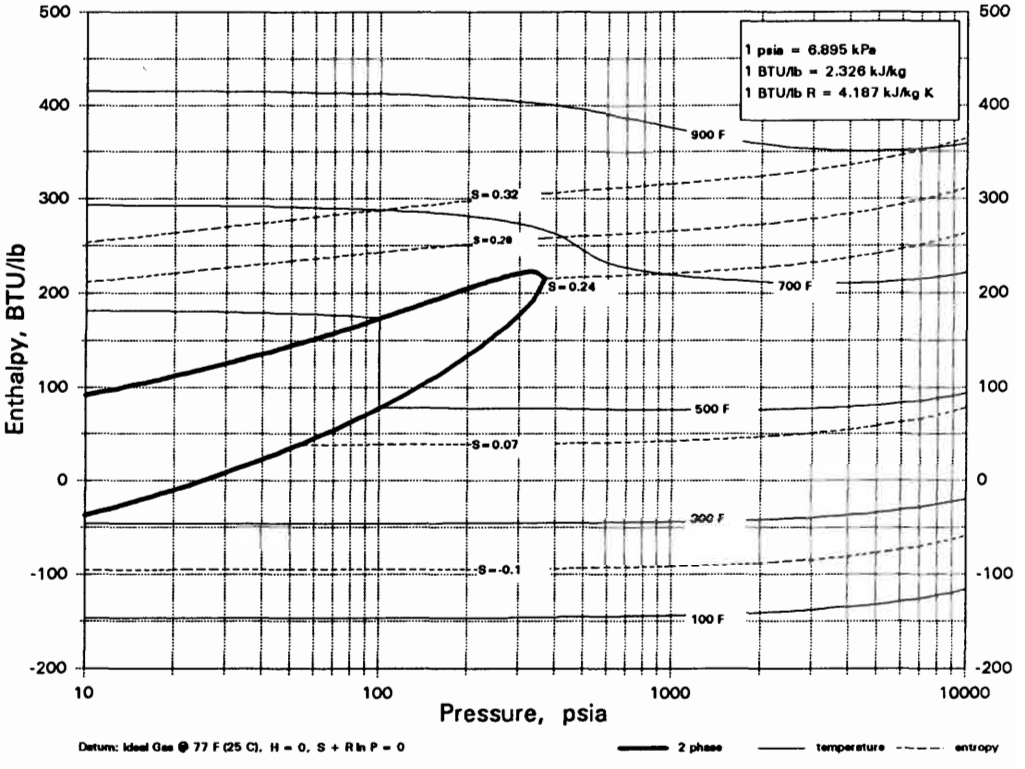
C8H16O2 n-BUTYL n-BUTYRATE



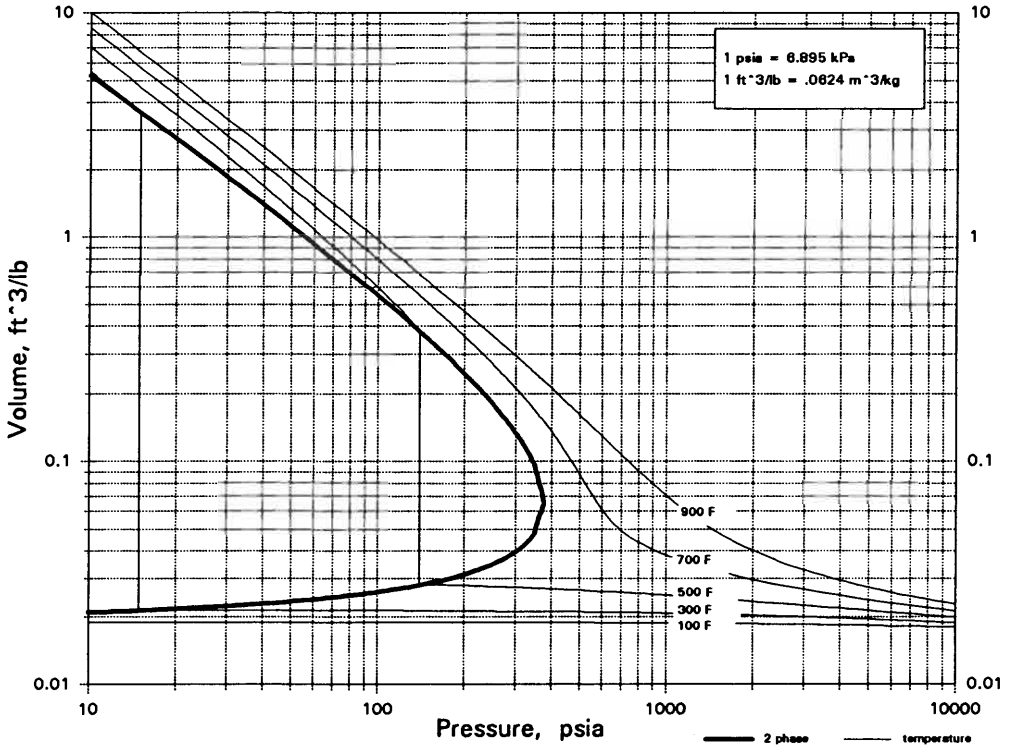


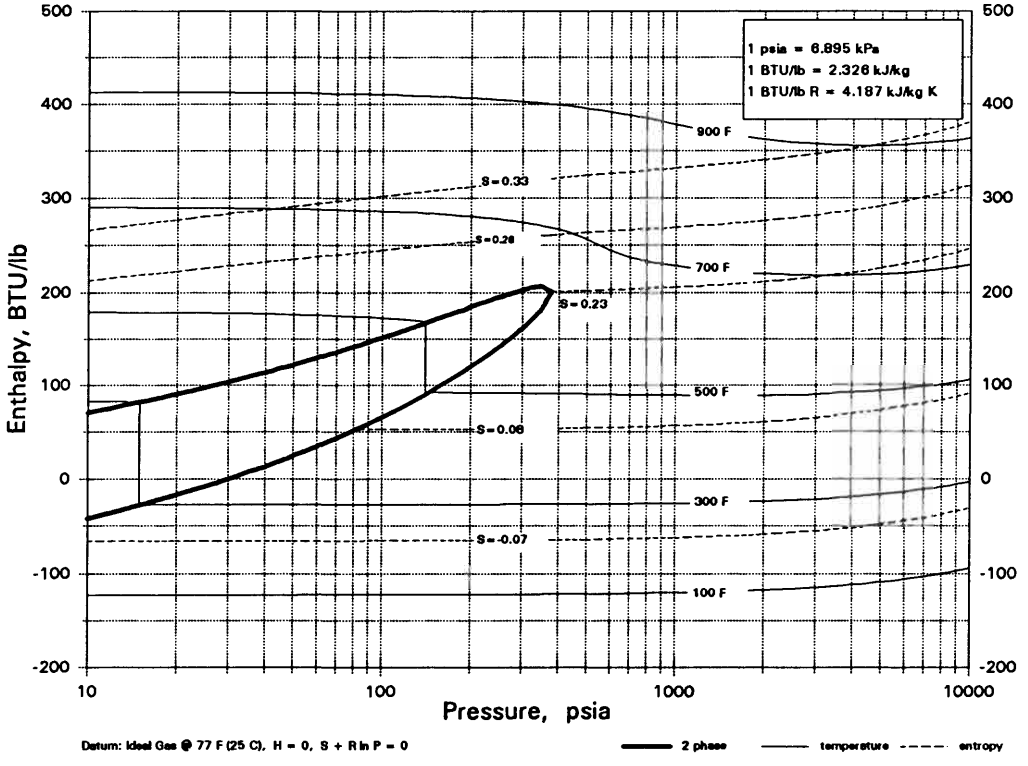
C8H16O2 n-HEXYL ACETATE



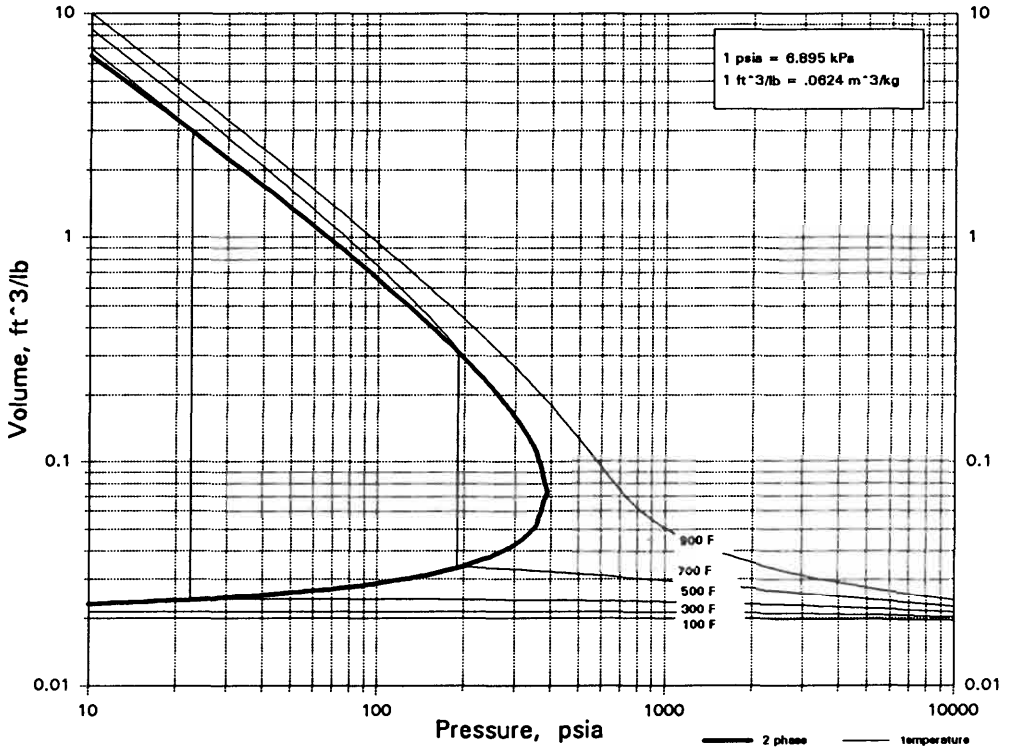


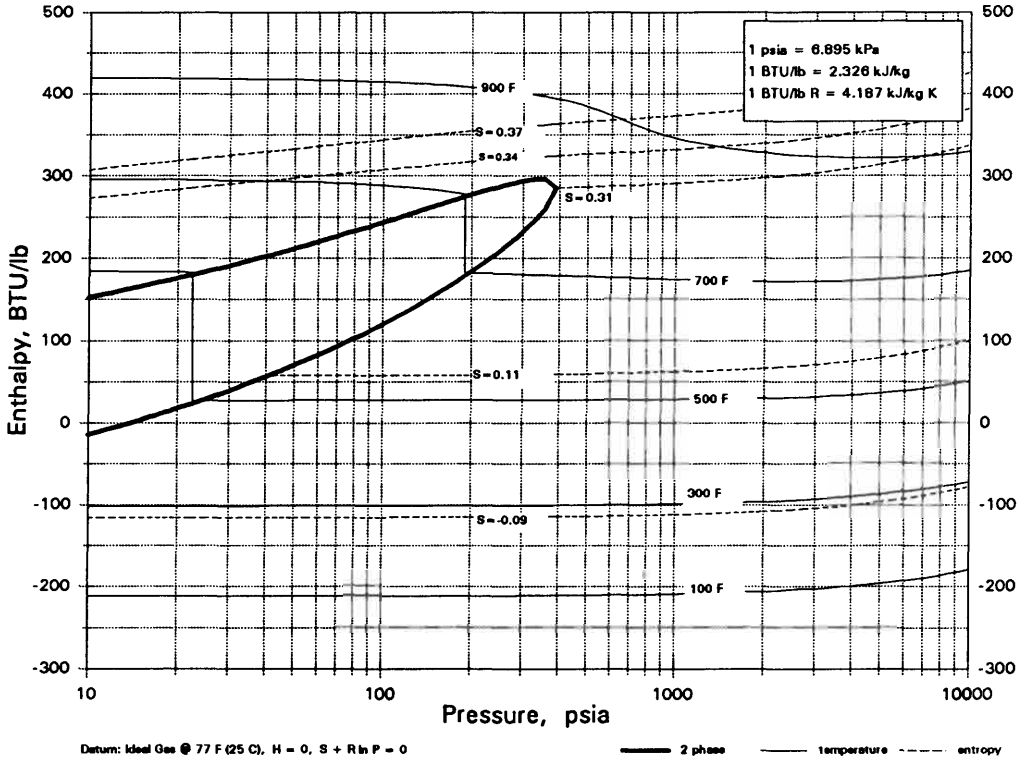
C8H16O2 ISOBUTYL ISOBUTYRATE



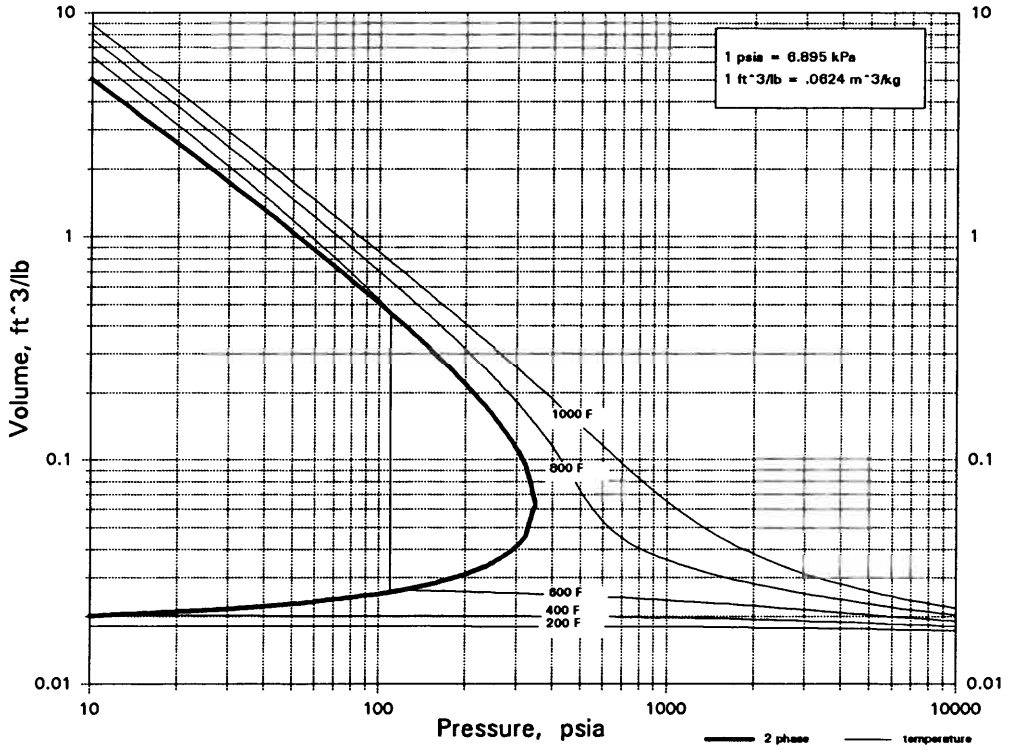


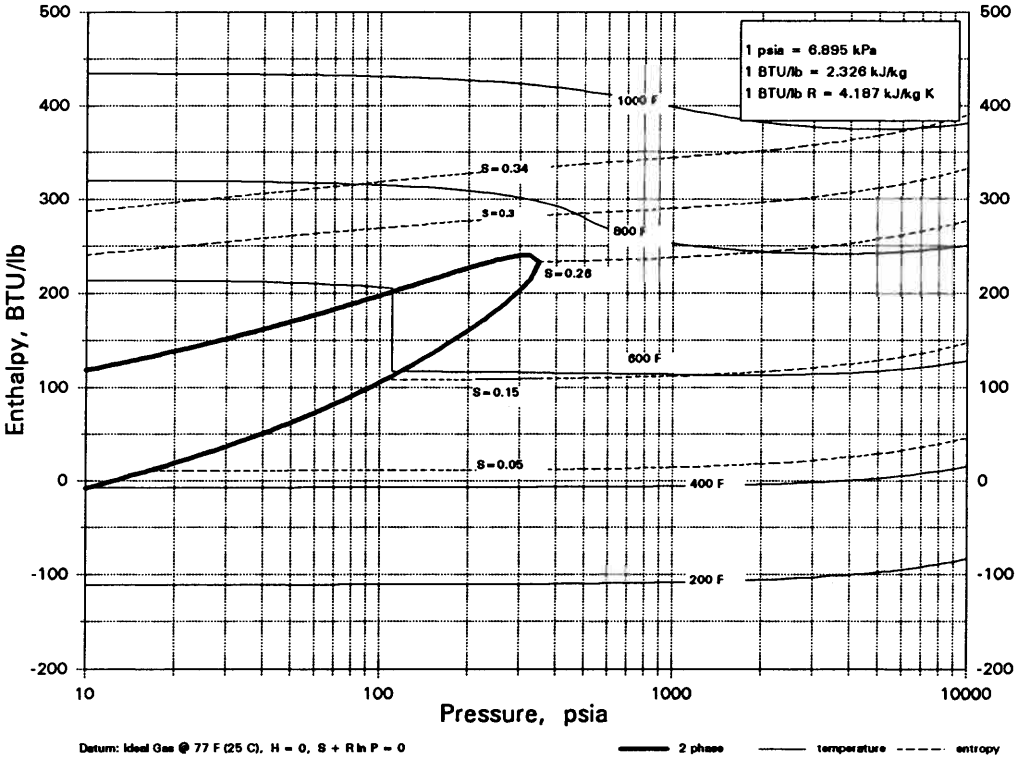
C8H16O2 n-OCTANOIC ACID



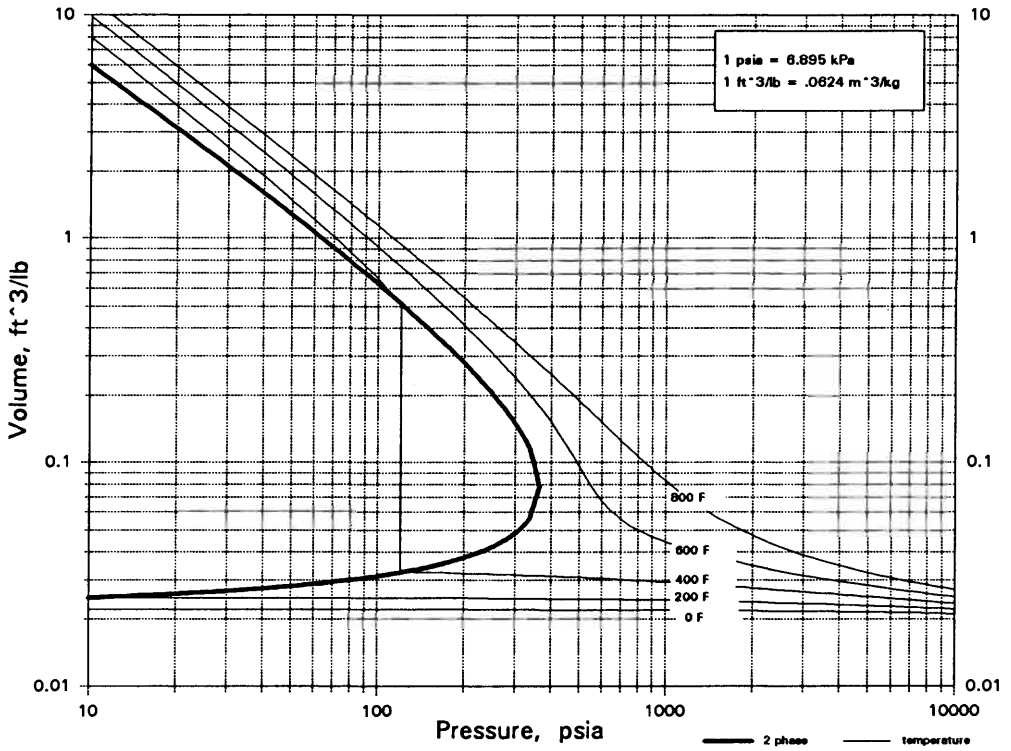


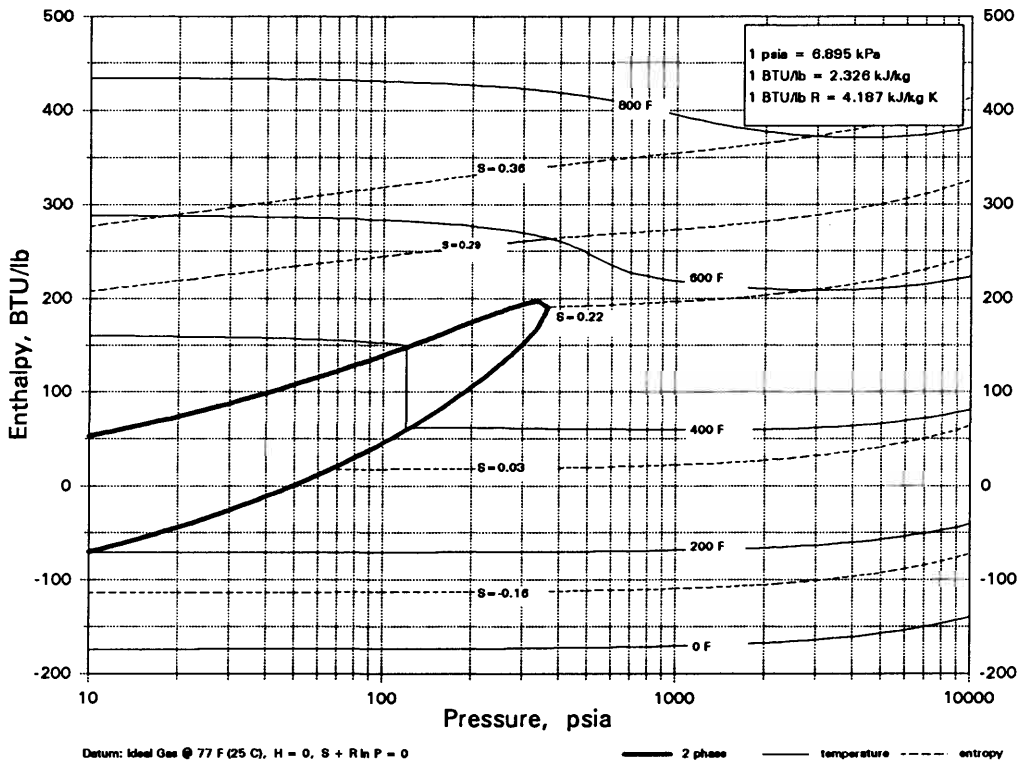
C8H16O4 DIETHYLENE GLYCOL ETHYL ETHER ACETATE



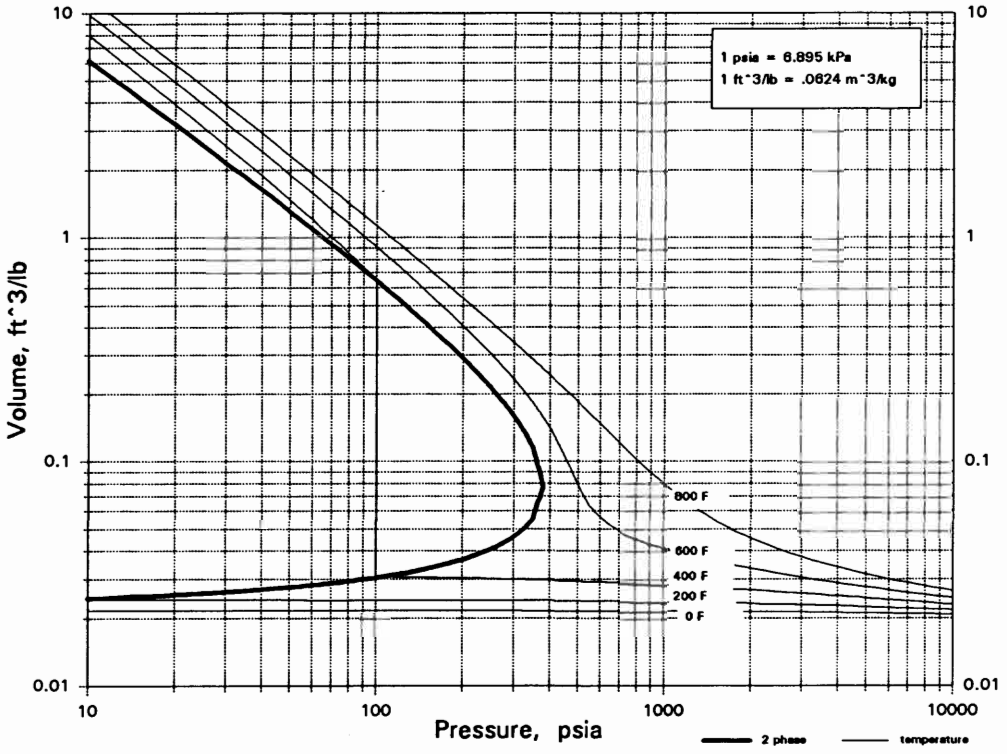


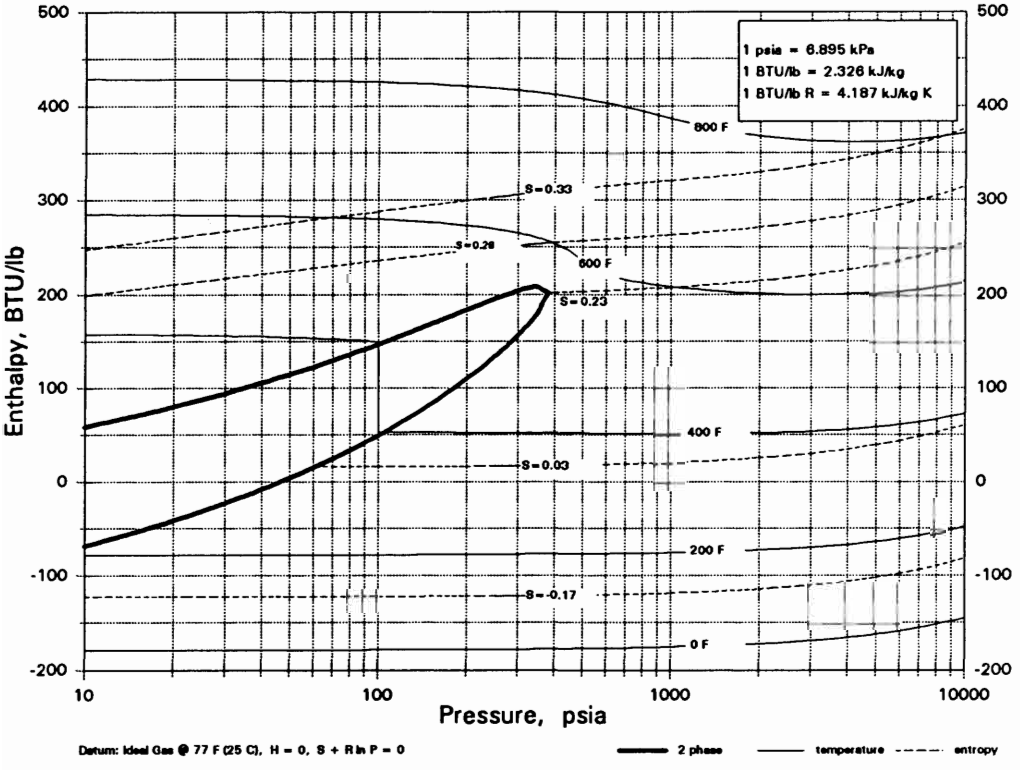
C8H18 2-2-DIMETHYLHEXANE



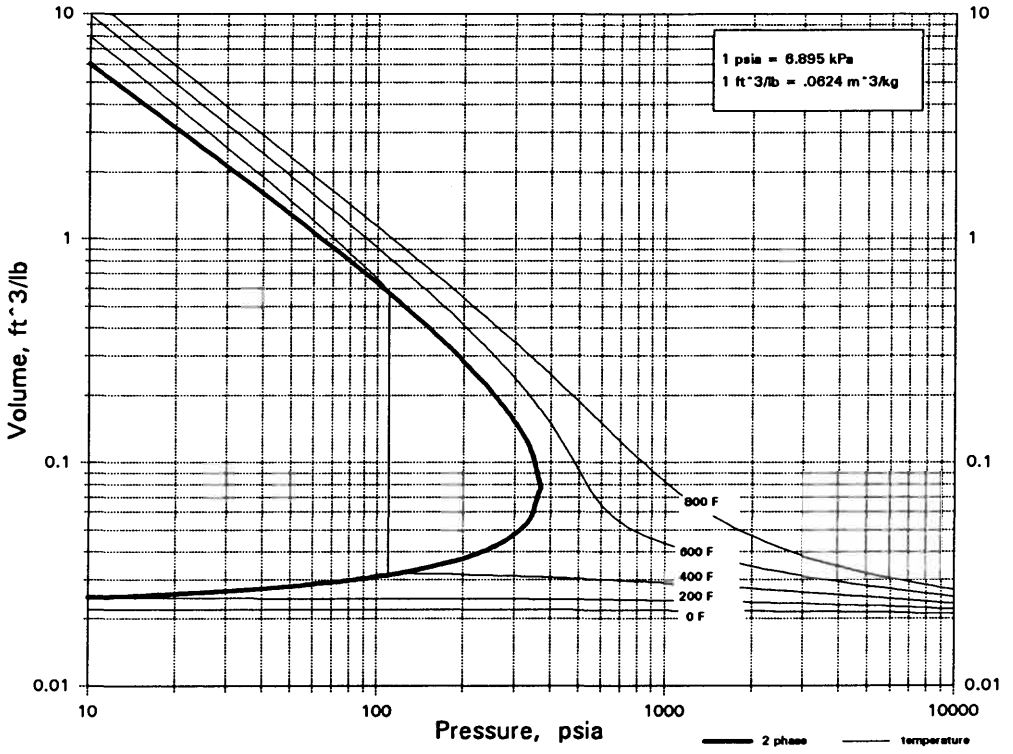


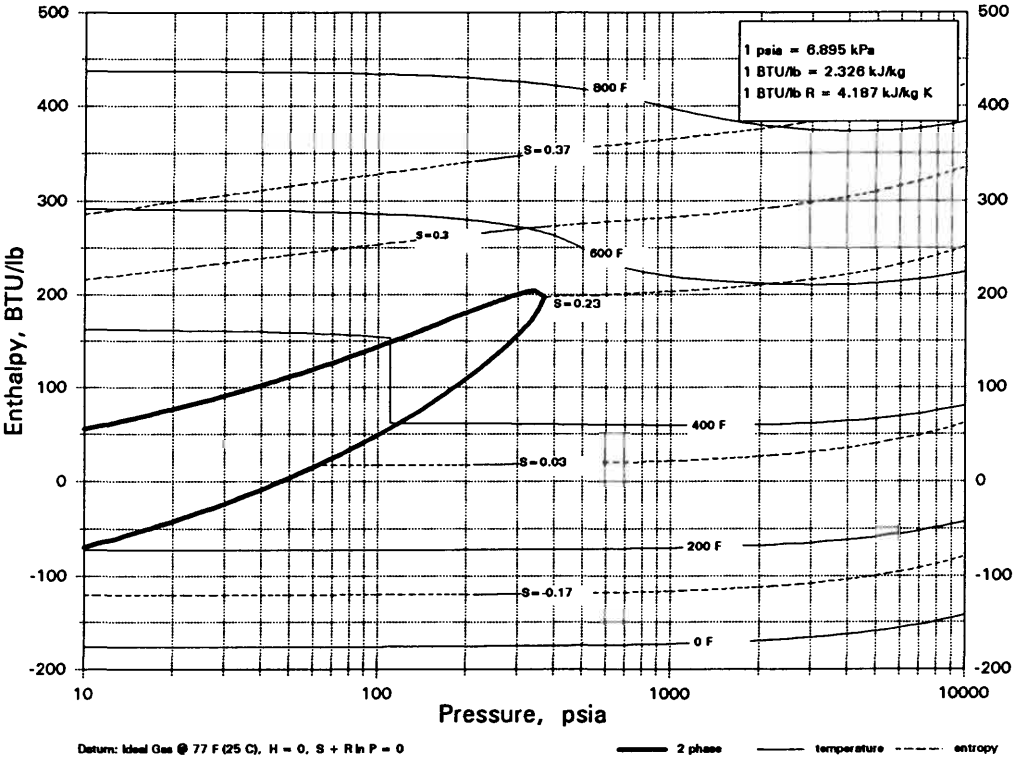
C8H18 2-3-DIMETHYLHEXANE



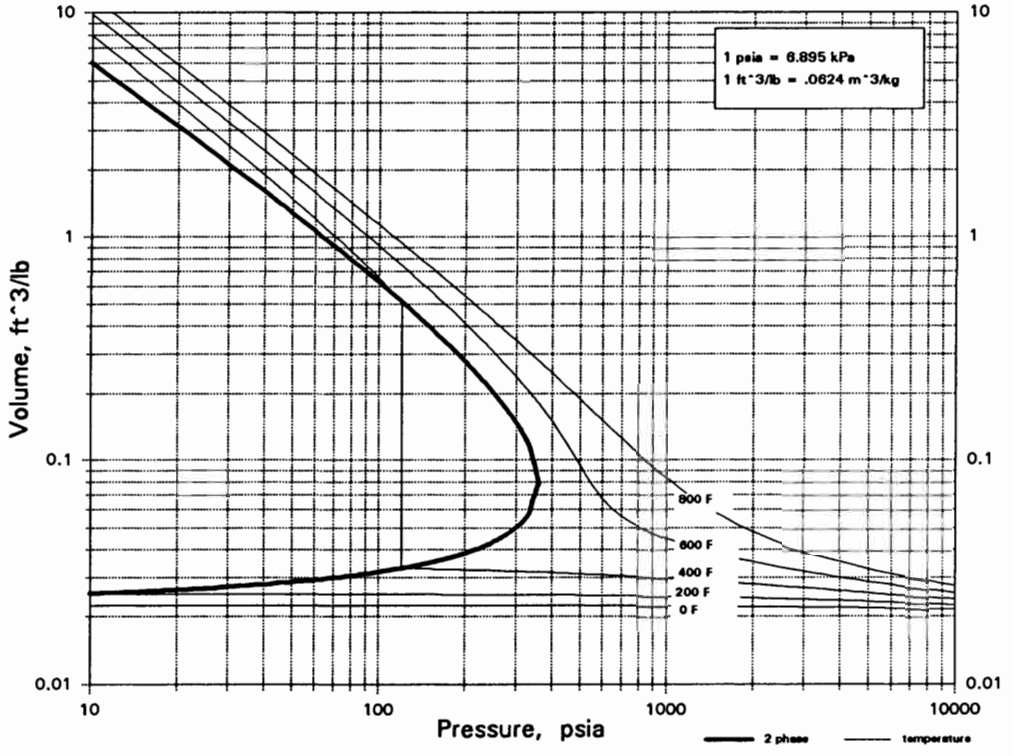


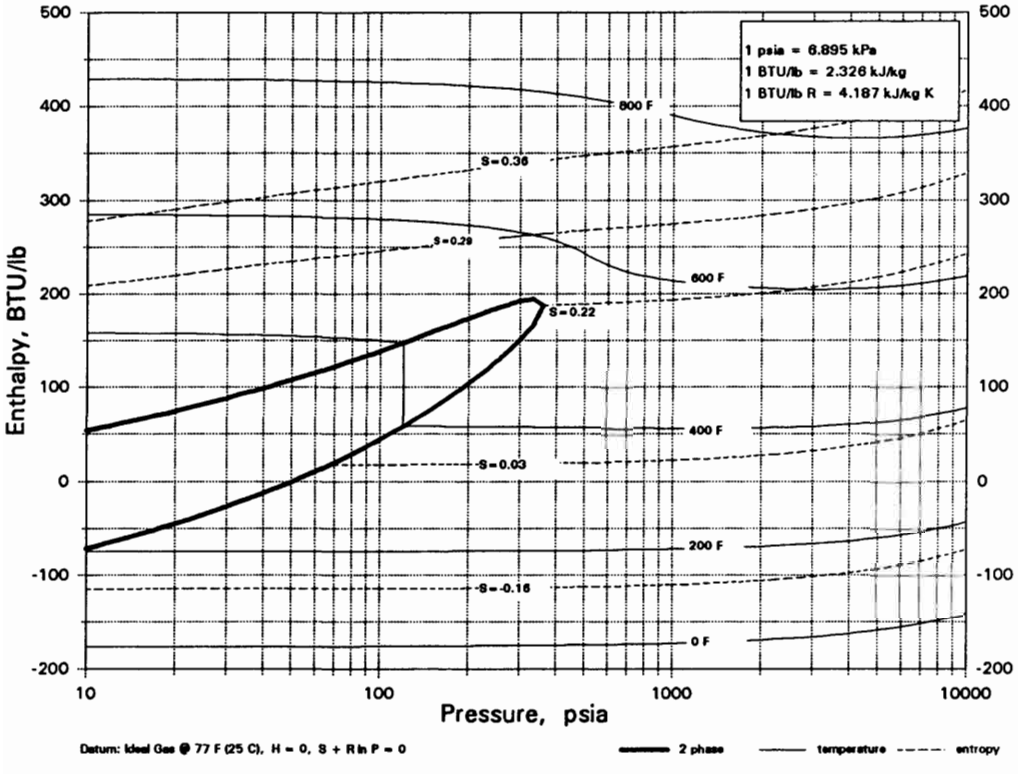
C8H18 2-4-DIMETHYLHEXANE



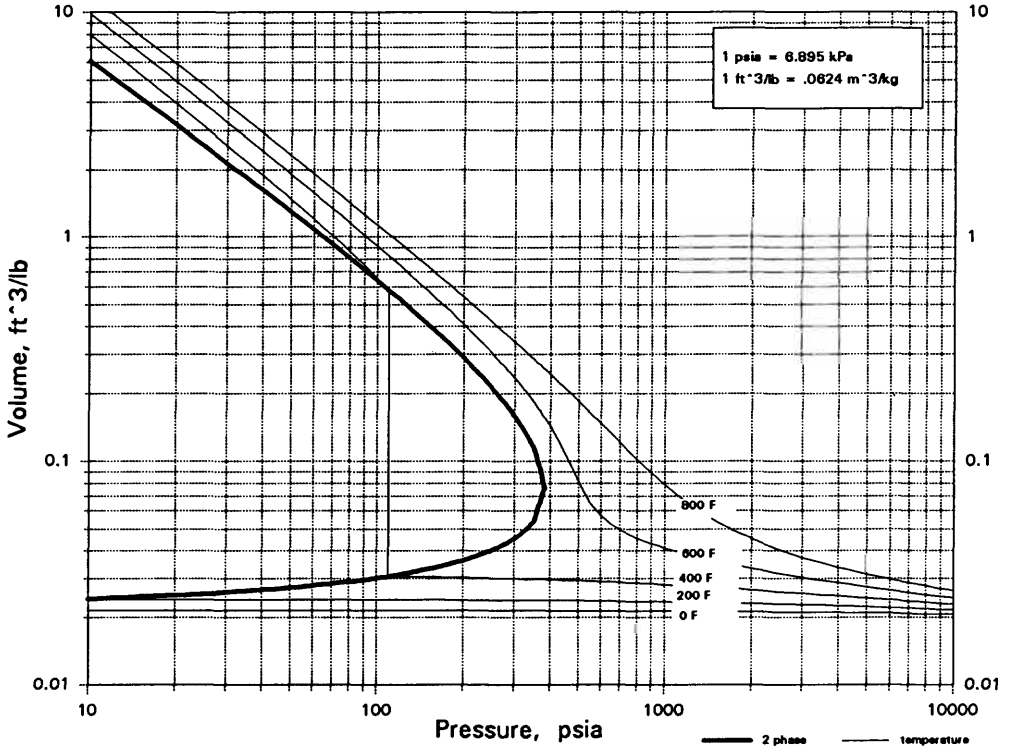


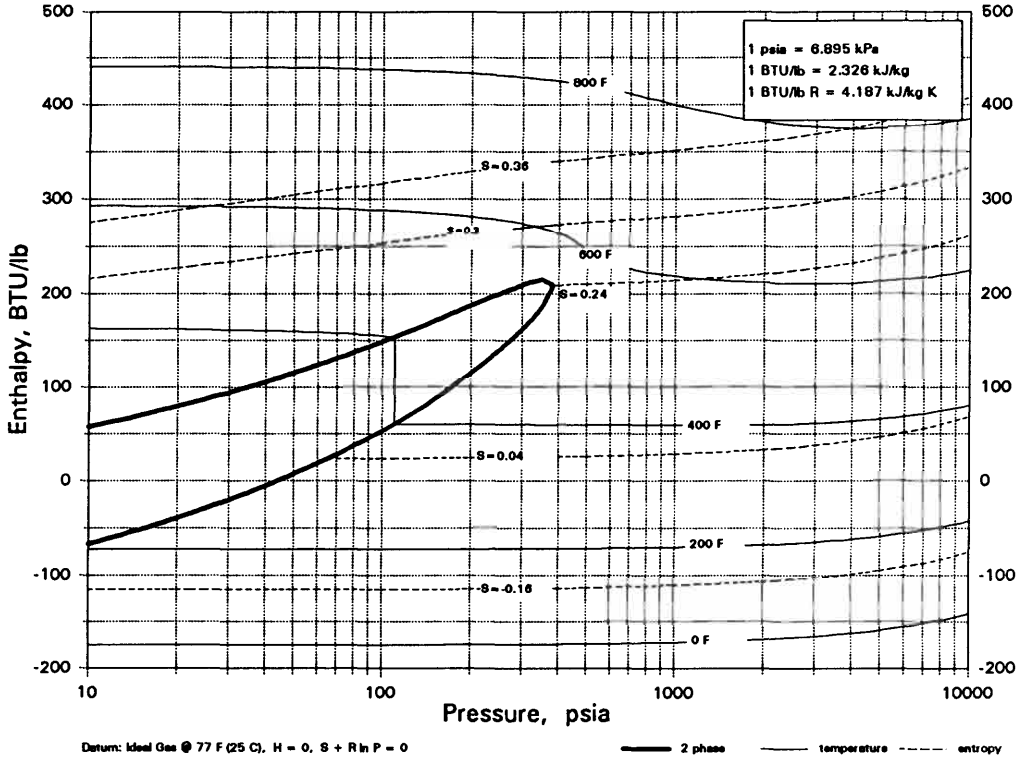
C8H18 2-5-DIMETHYLHEXANE



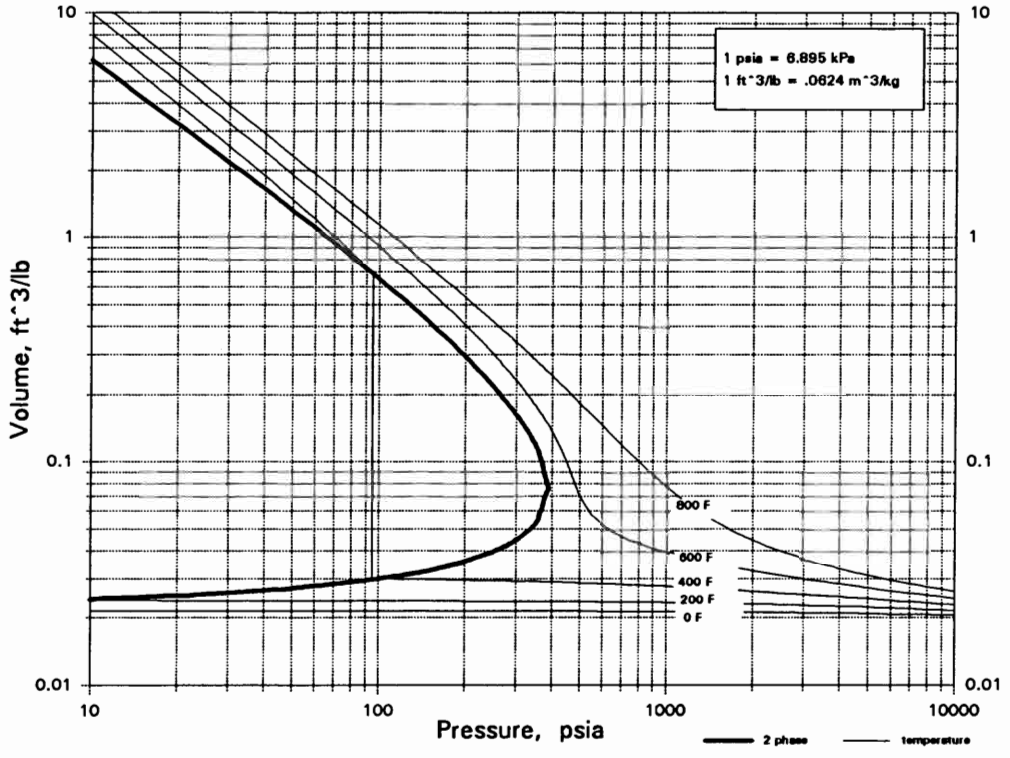


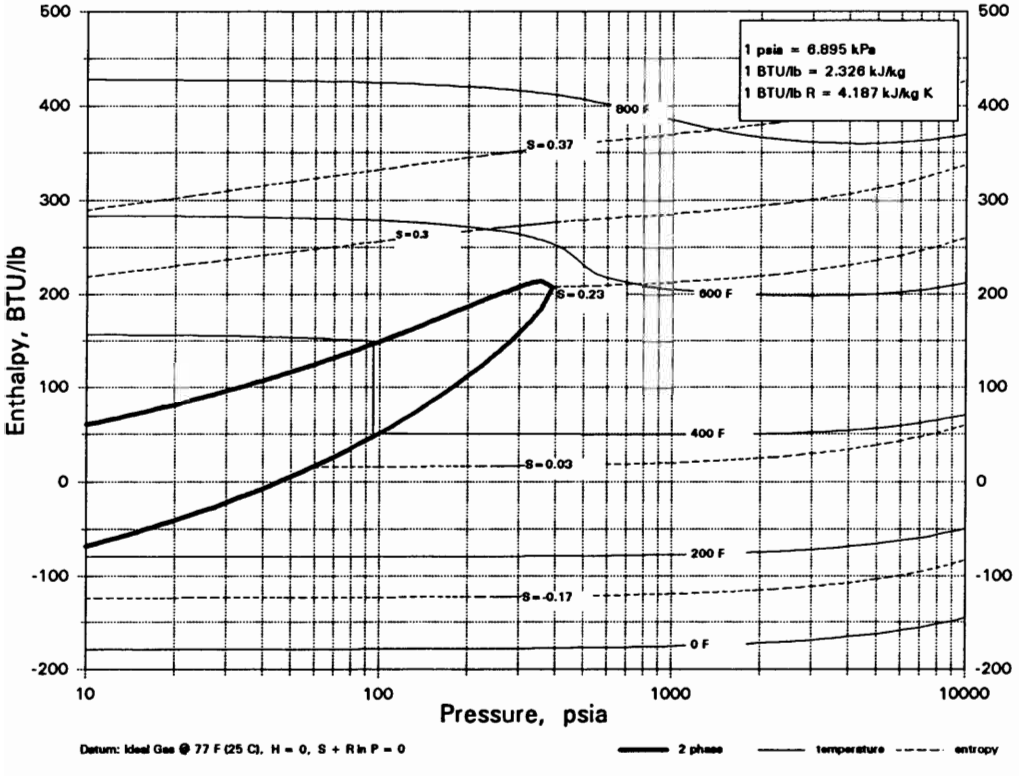
C8H18 3-3-DIMETHYLHEXANE



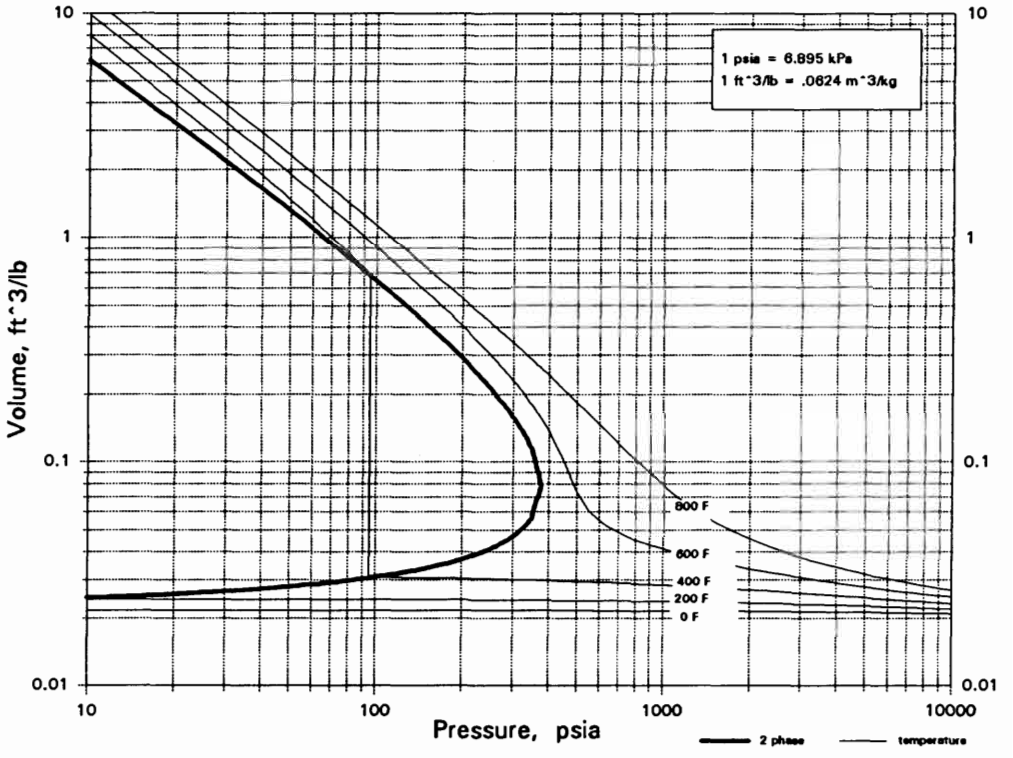


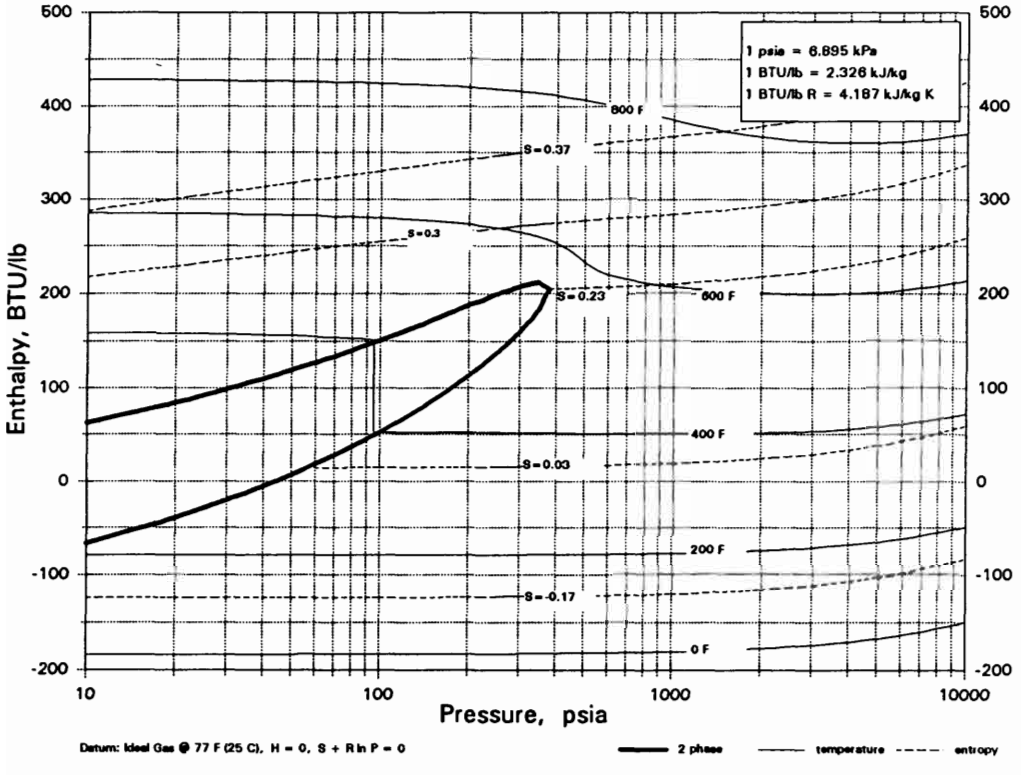
C8H18 3-4-DIMETHYLHEXANE



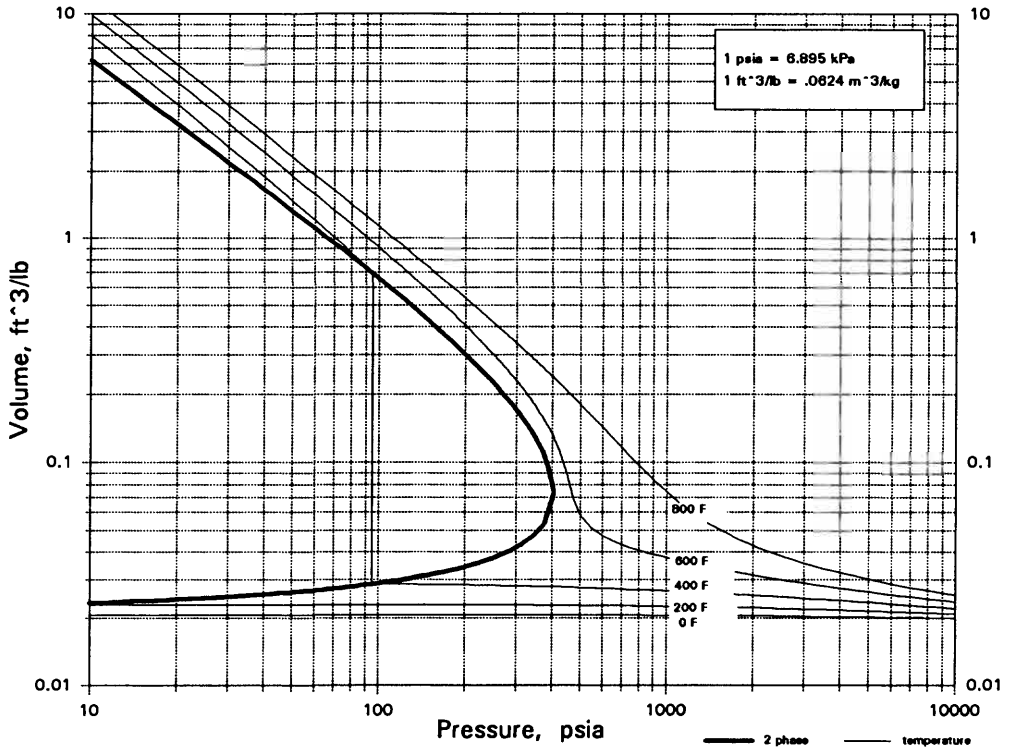


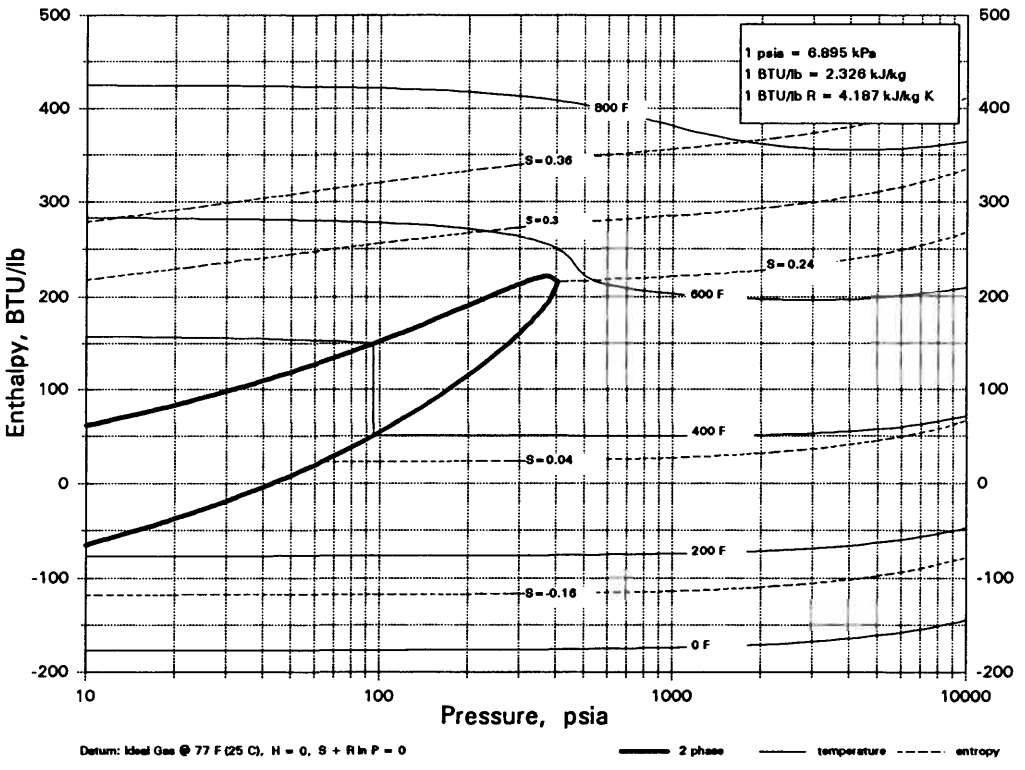
C8H18 3-ETHYLHEXANE



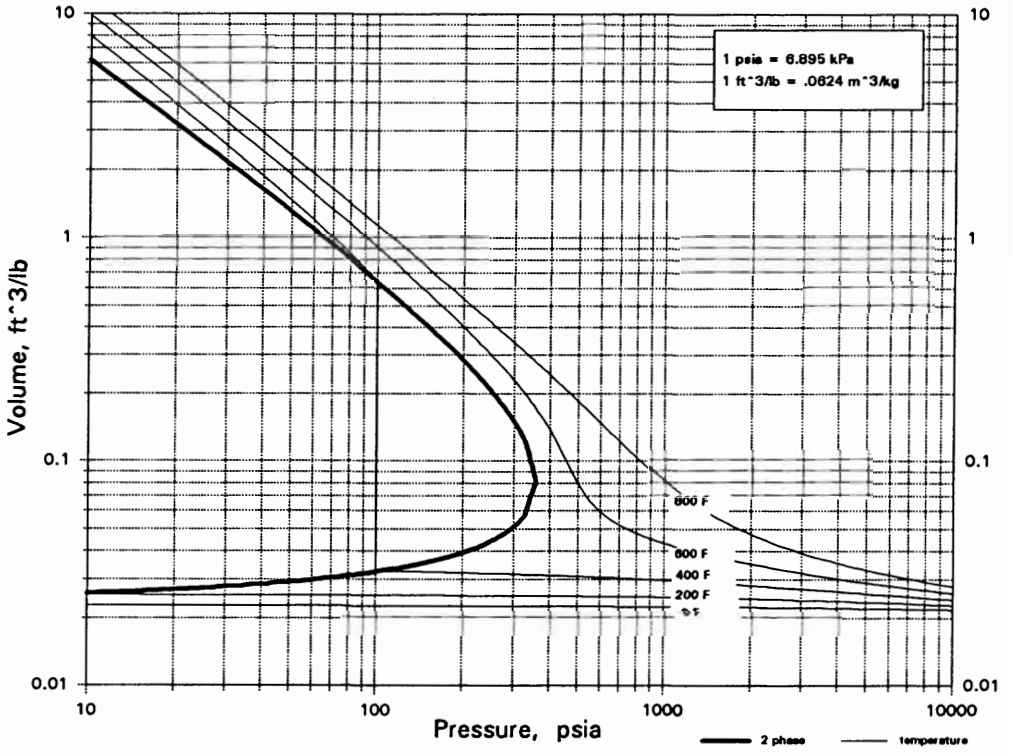


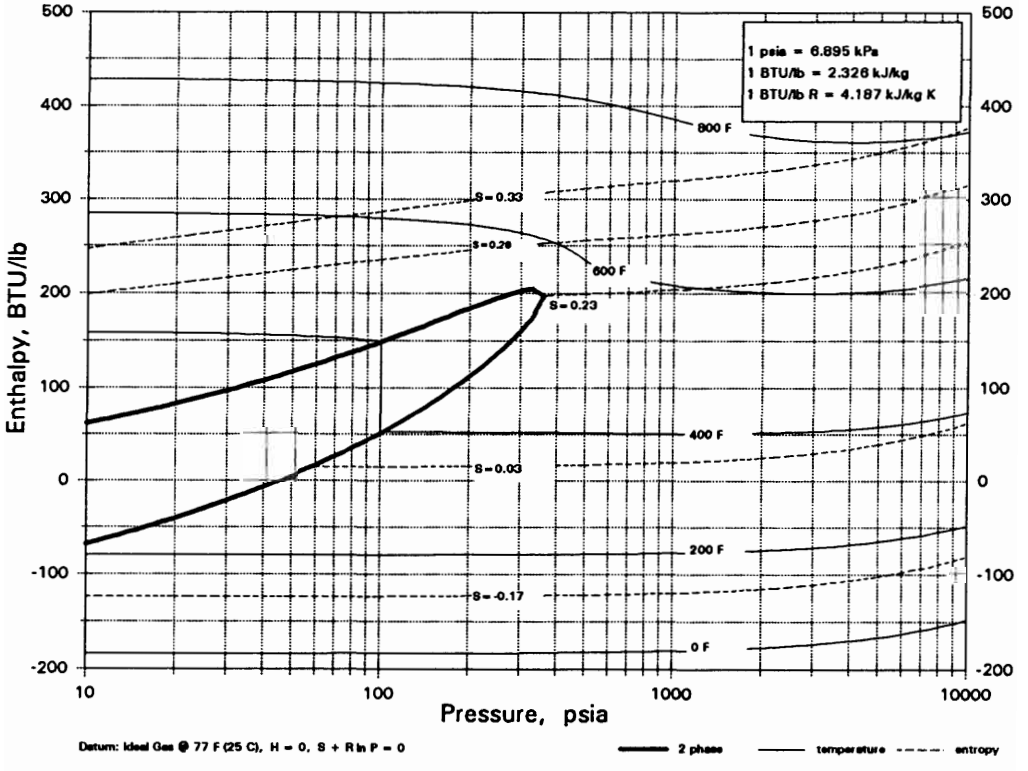
C8H18	3-METHYL-3-ETHYLPENTANE



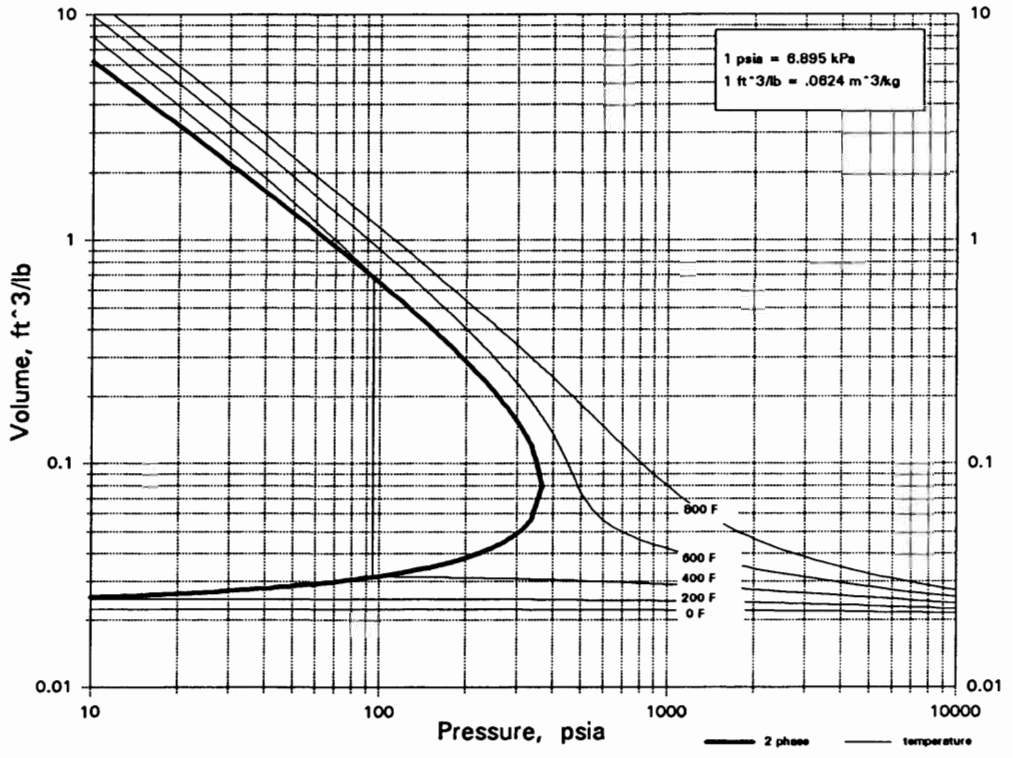


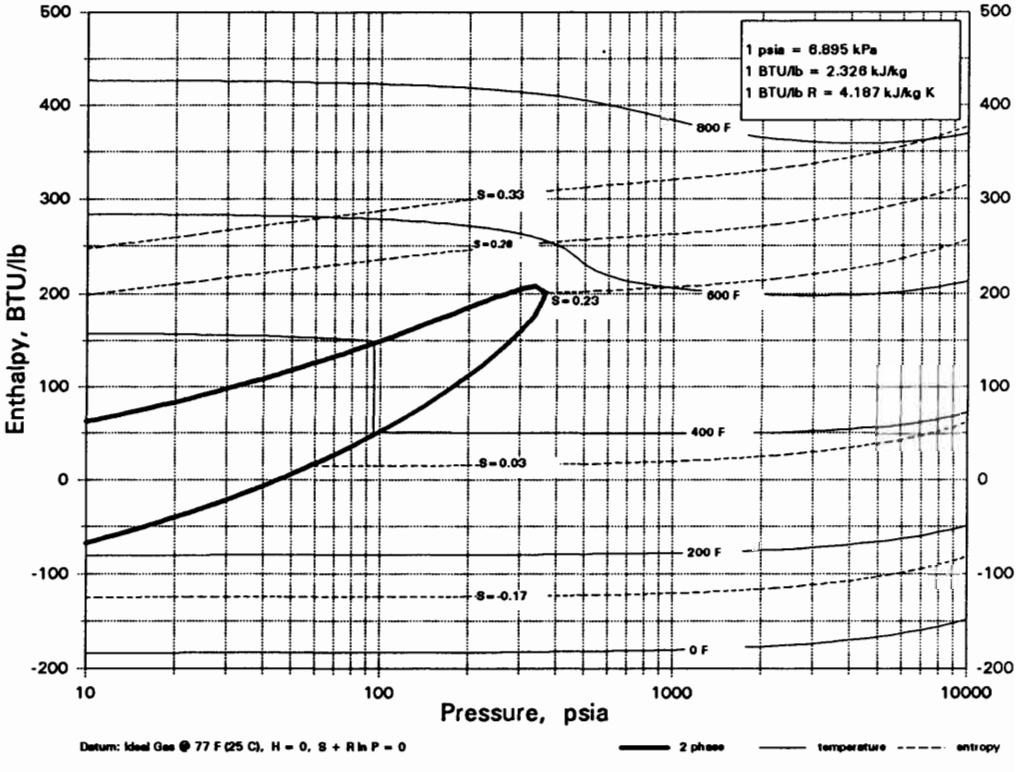
C8H18 2-METHYLHEPTANE



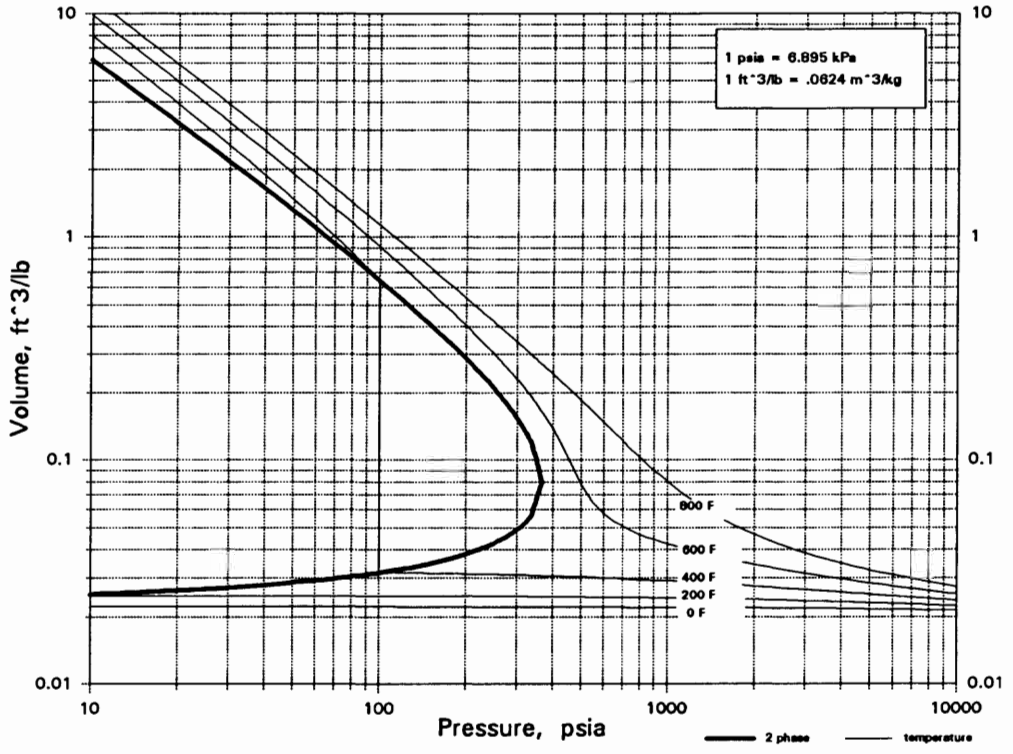


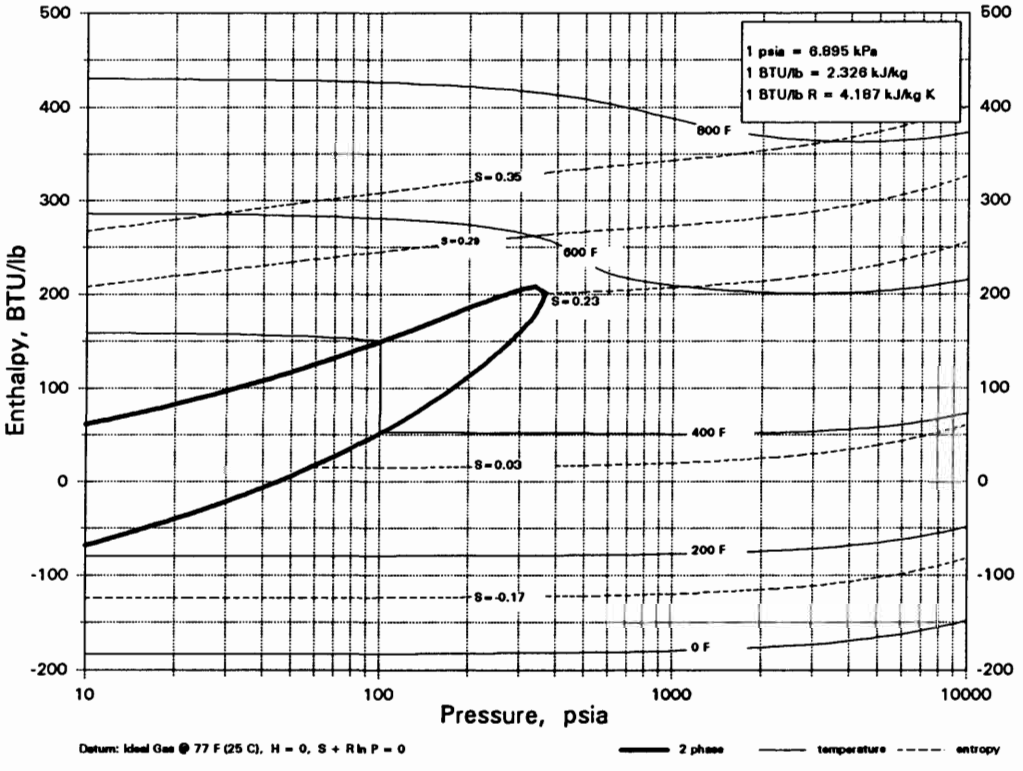
C8H18 3-METHYLHEPTANE



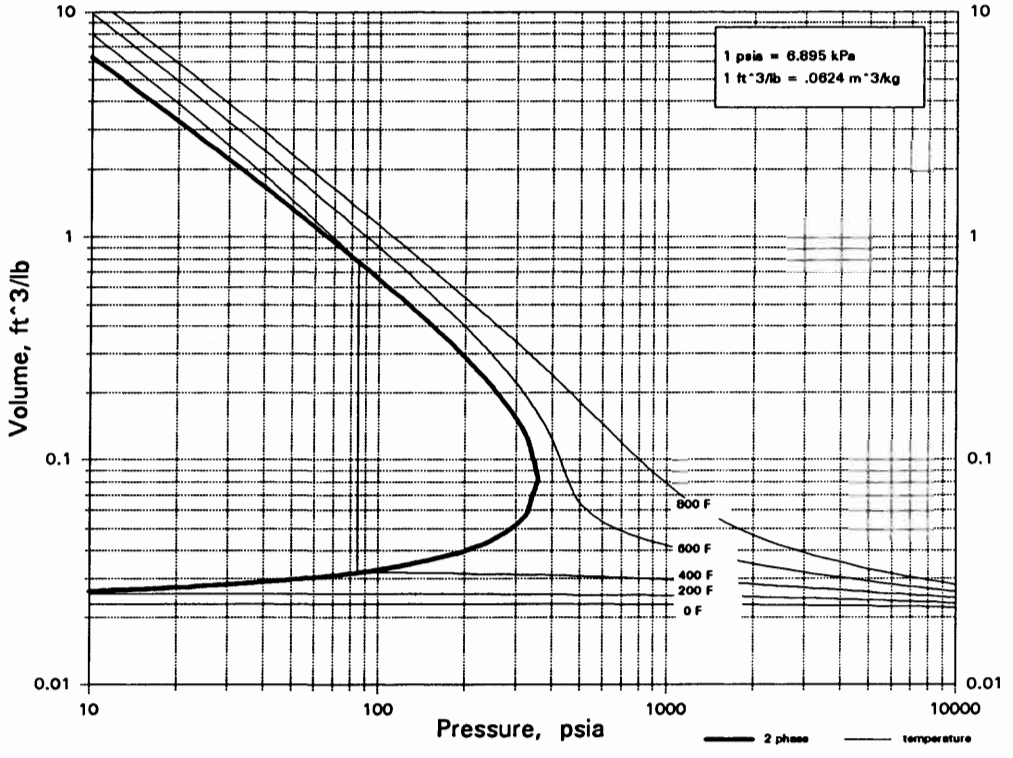


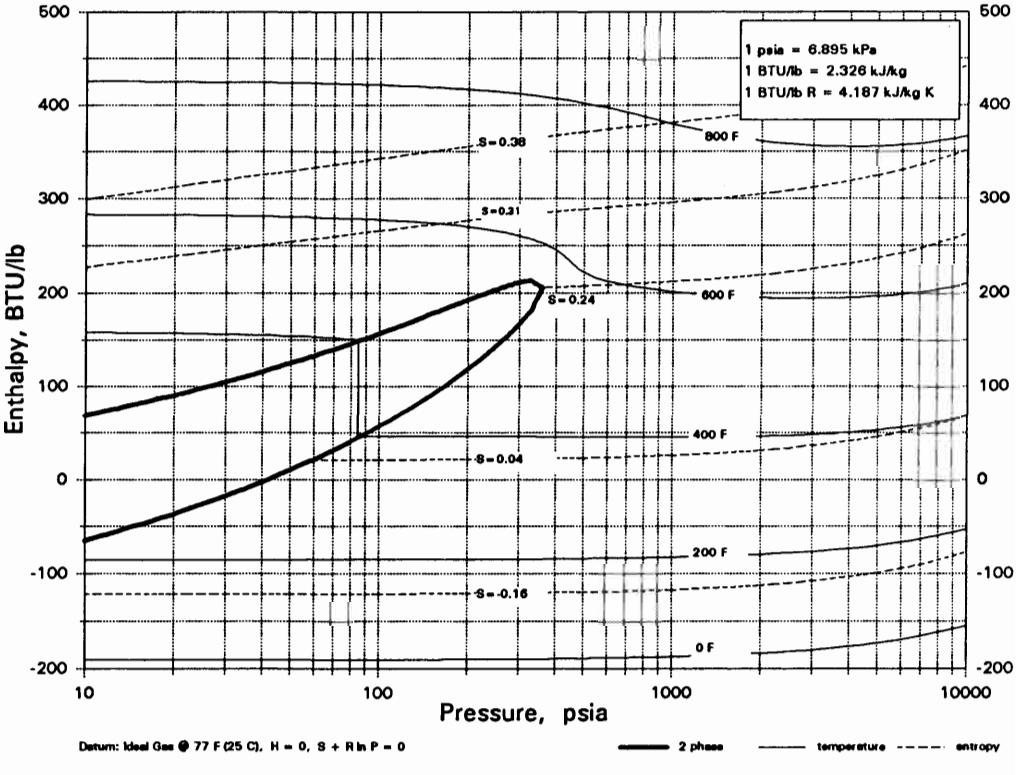
C8H18 4-METHYLHEPTANE



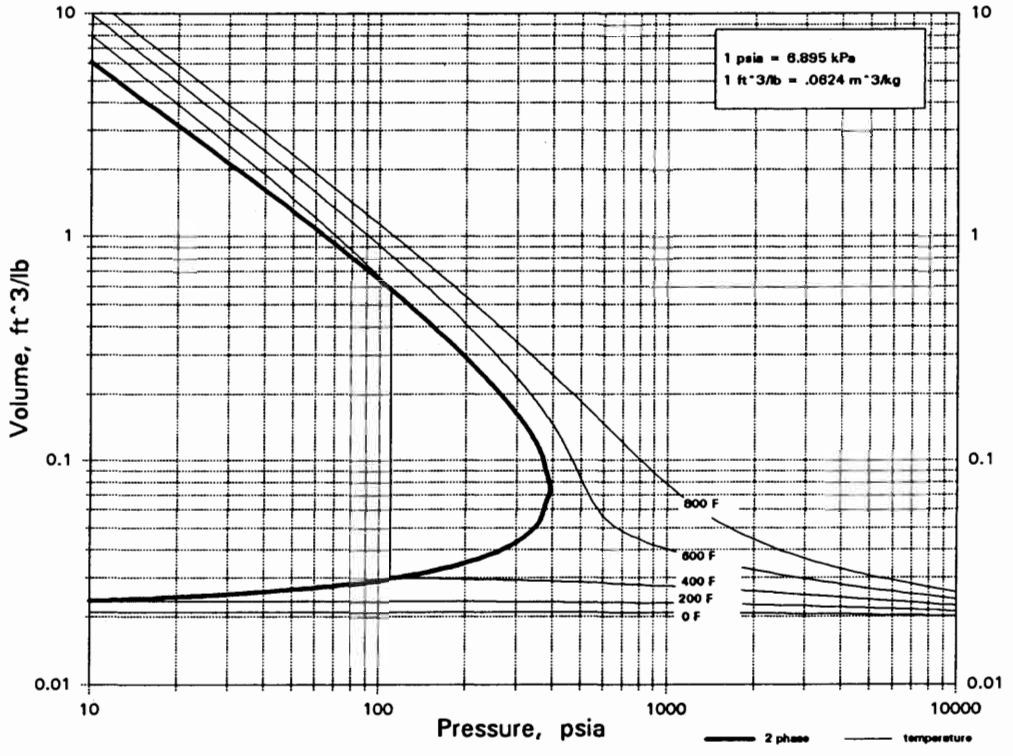


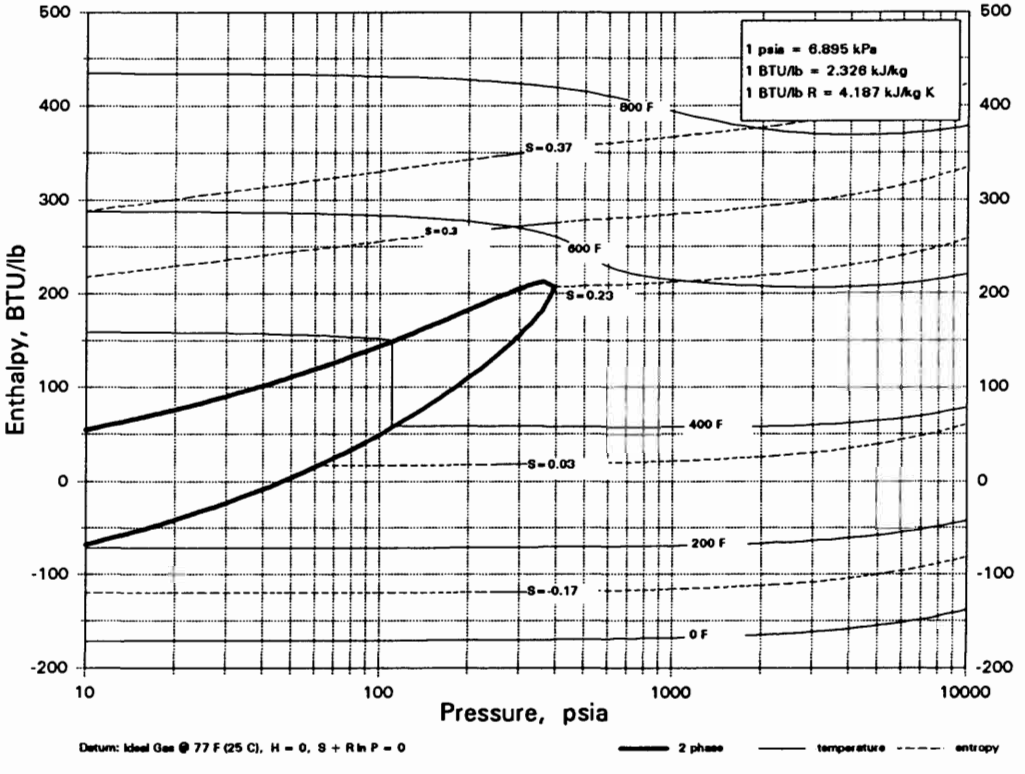
C8H18 n-OCTANE



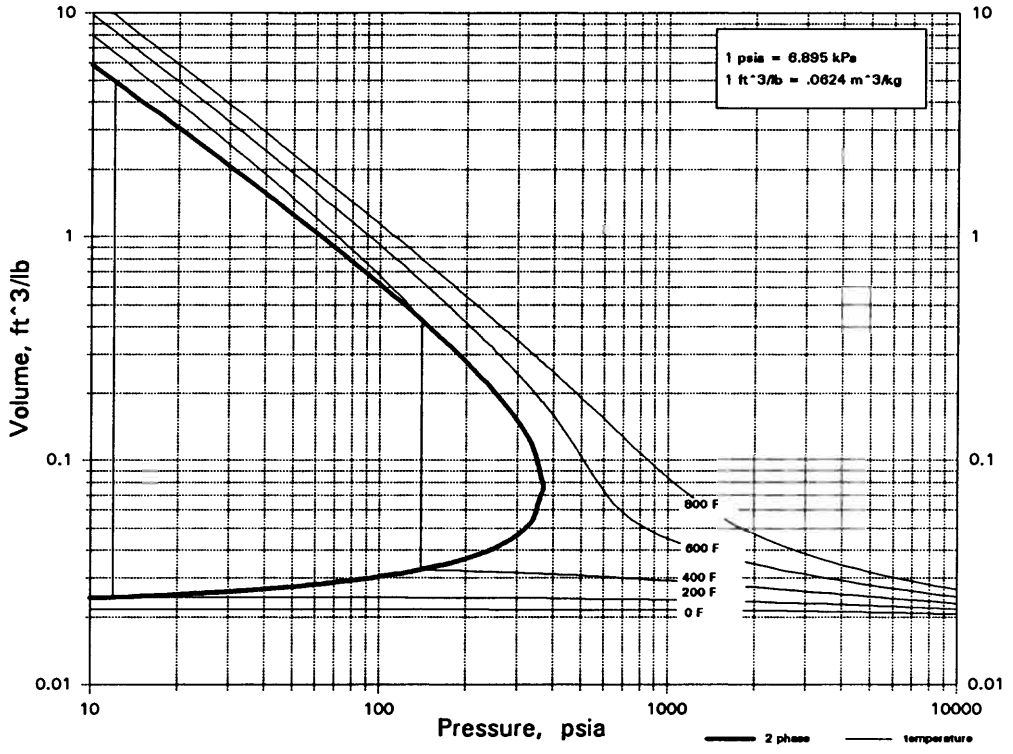


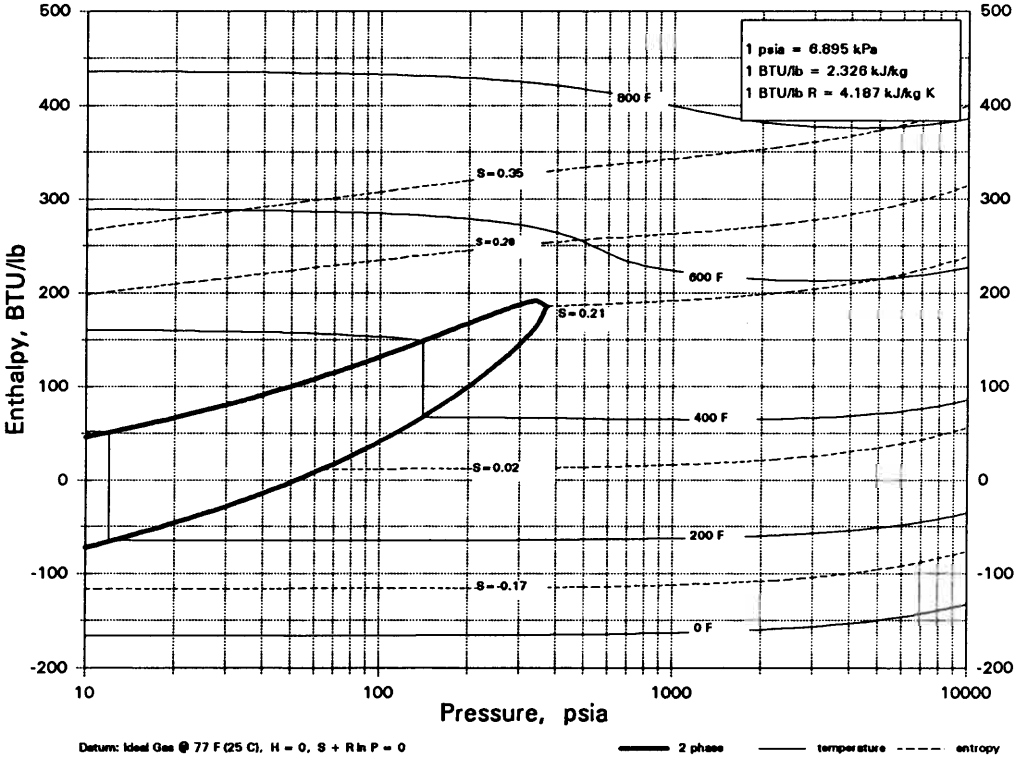
C8H18 2-2-3-TRIMETHYLPENTANE



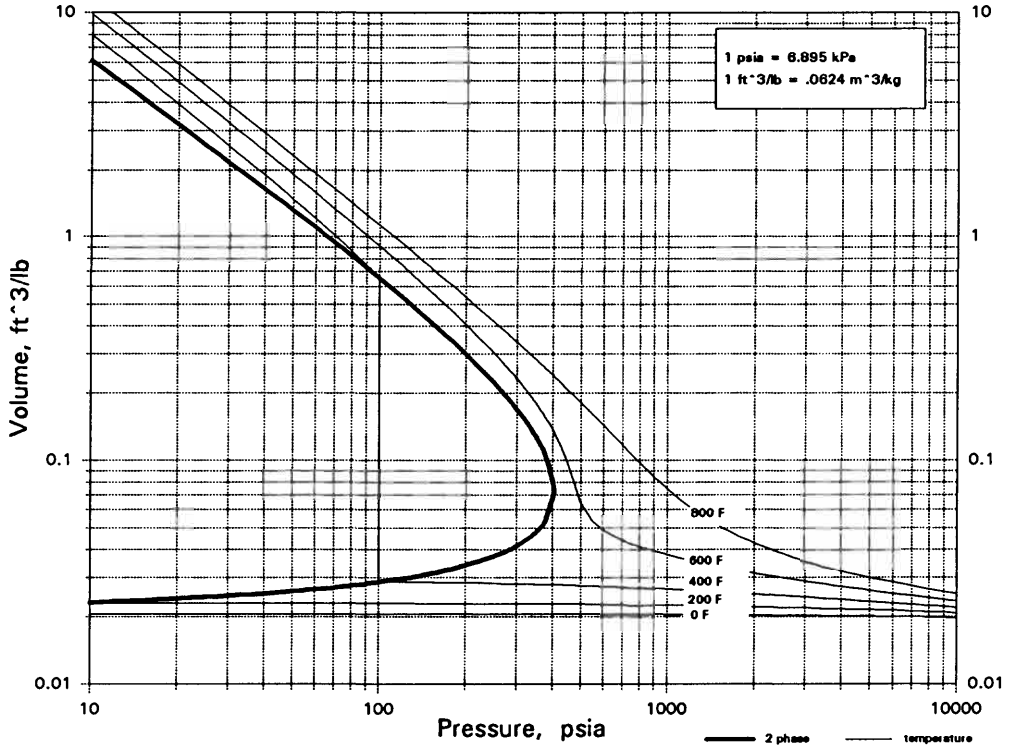


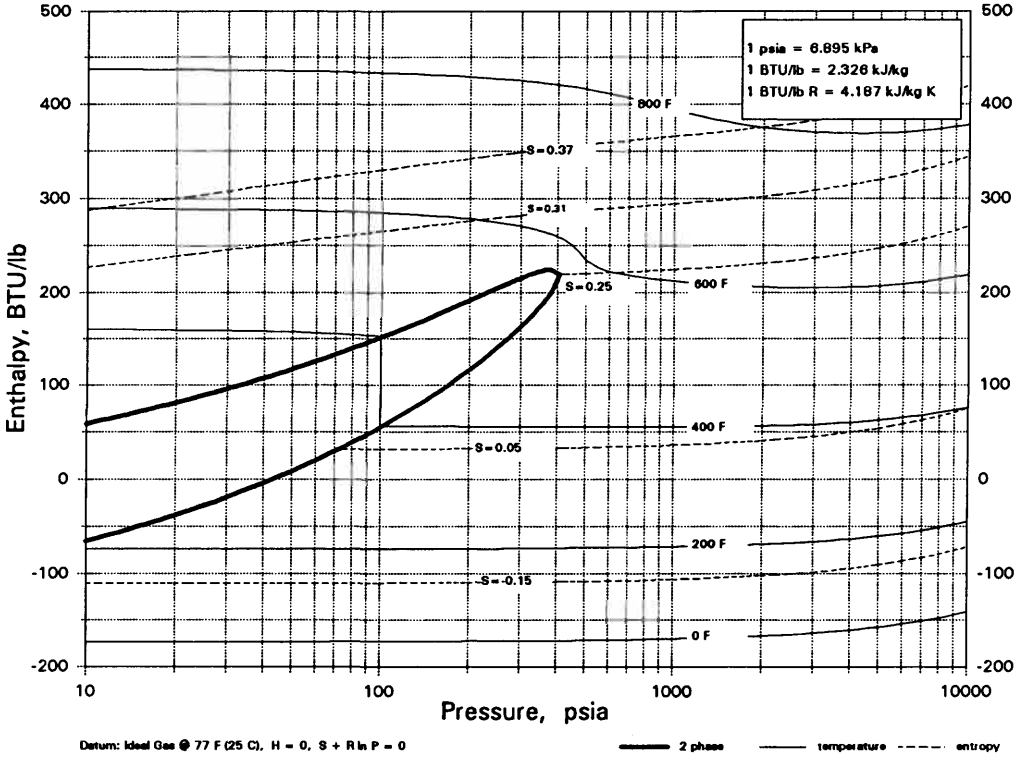
C8H18 2-2-4-TRIMETHYLPENTANE





C8H18 2-3-3-TRIMETHYLPENTANE





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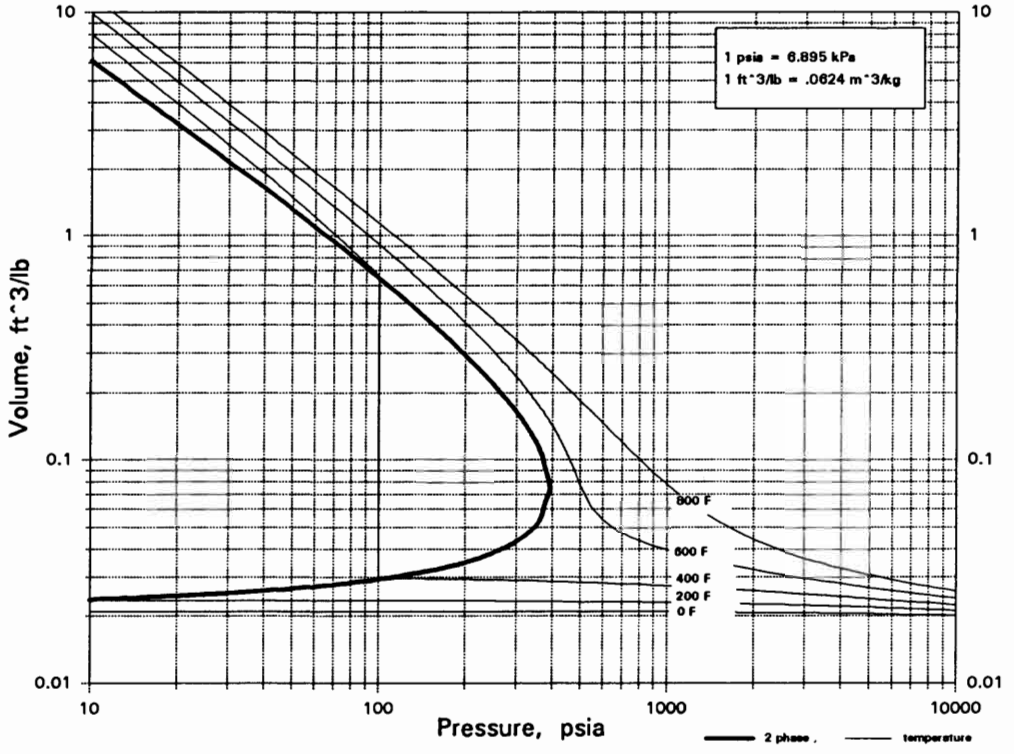
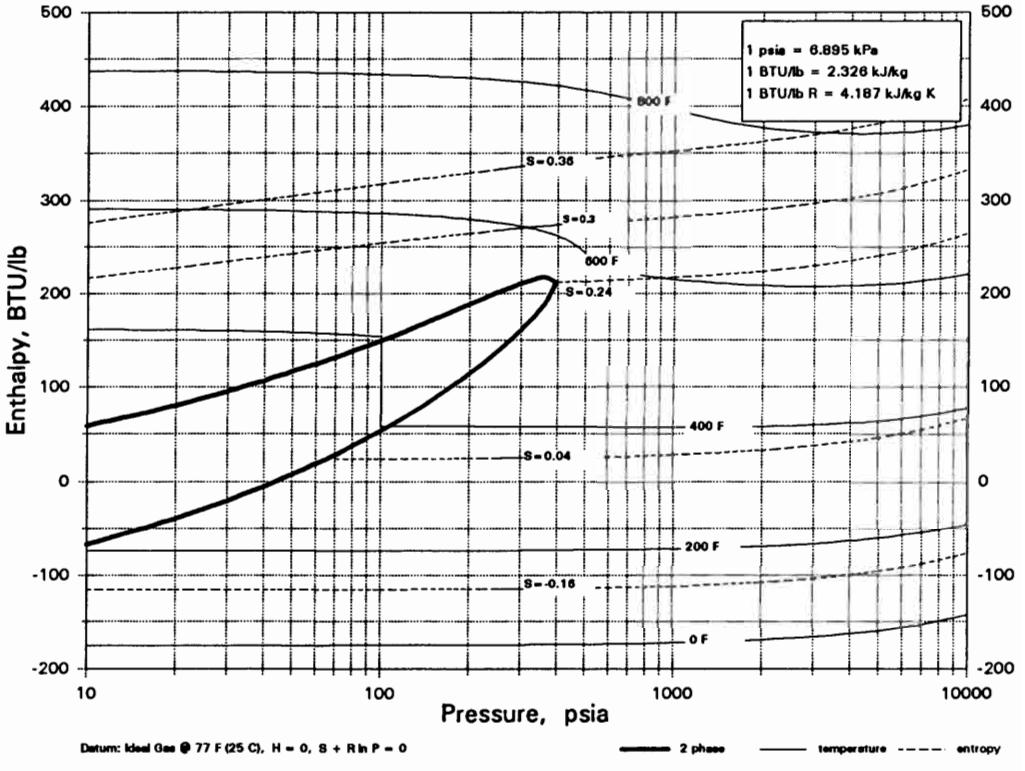
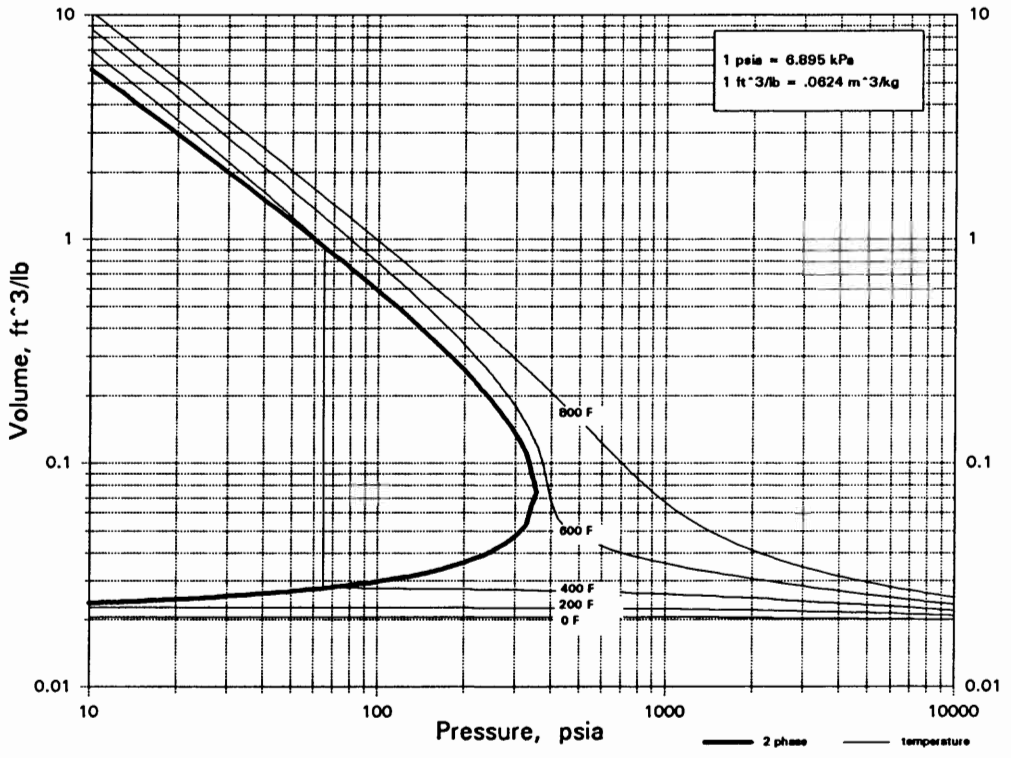
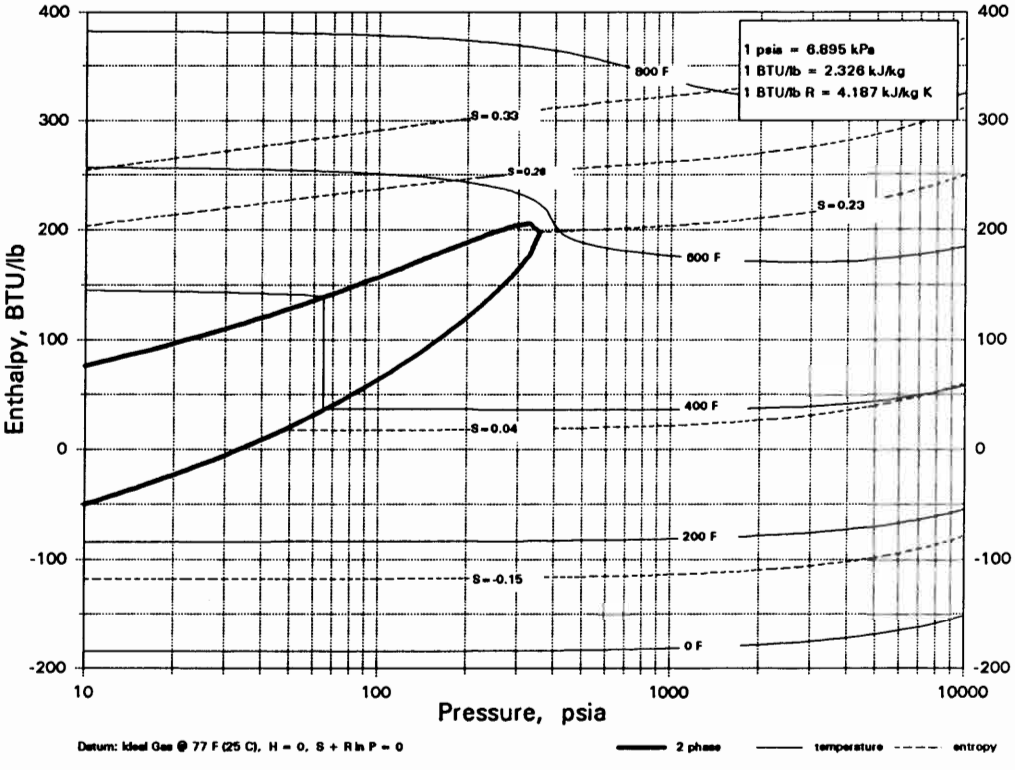


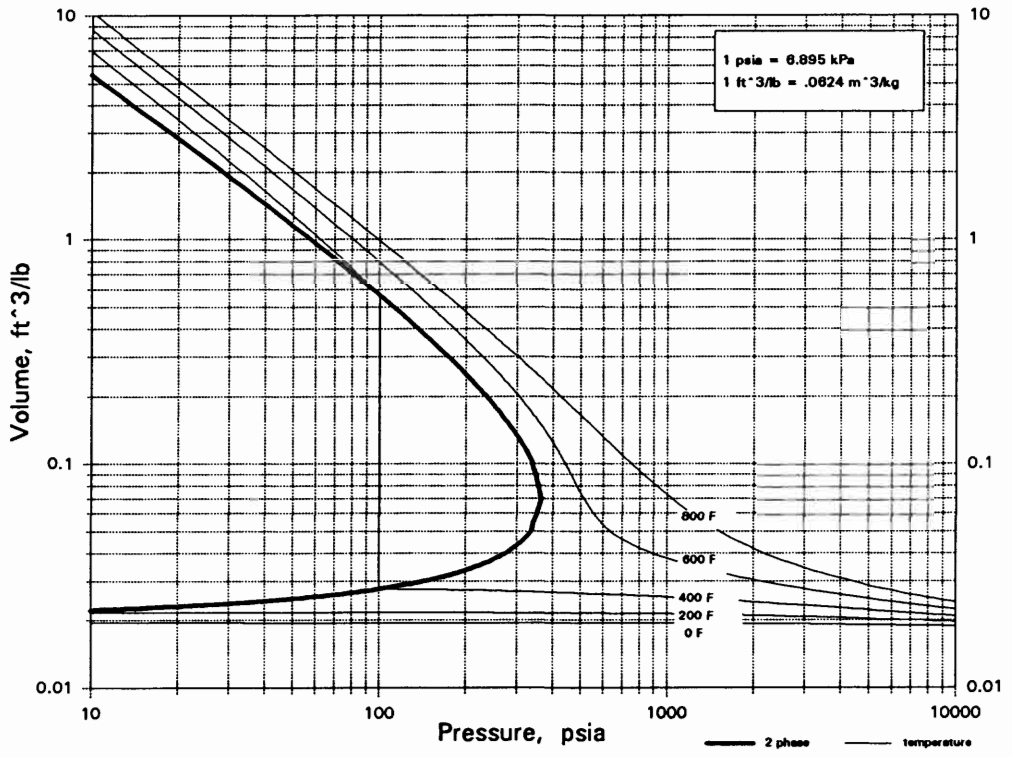


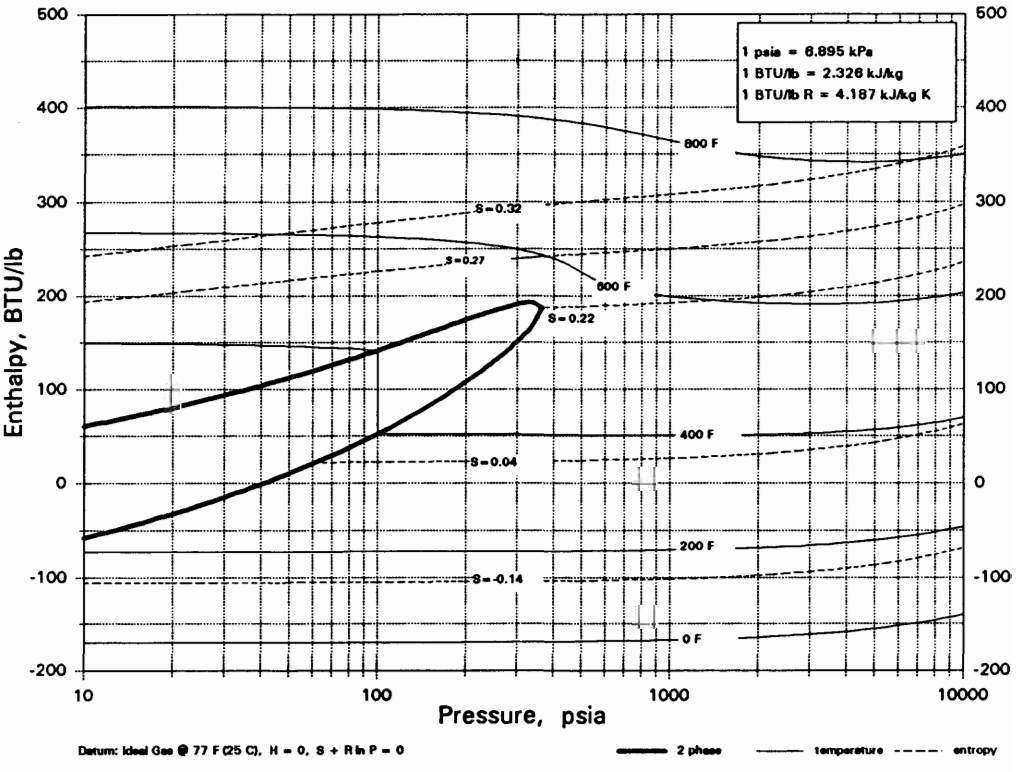
C8H18O DI-n-BUTYL ETHER



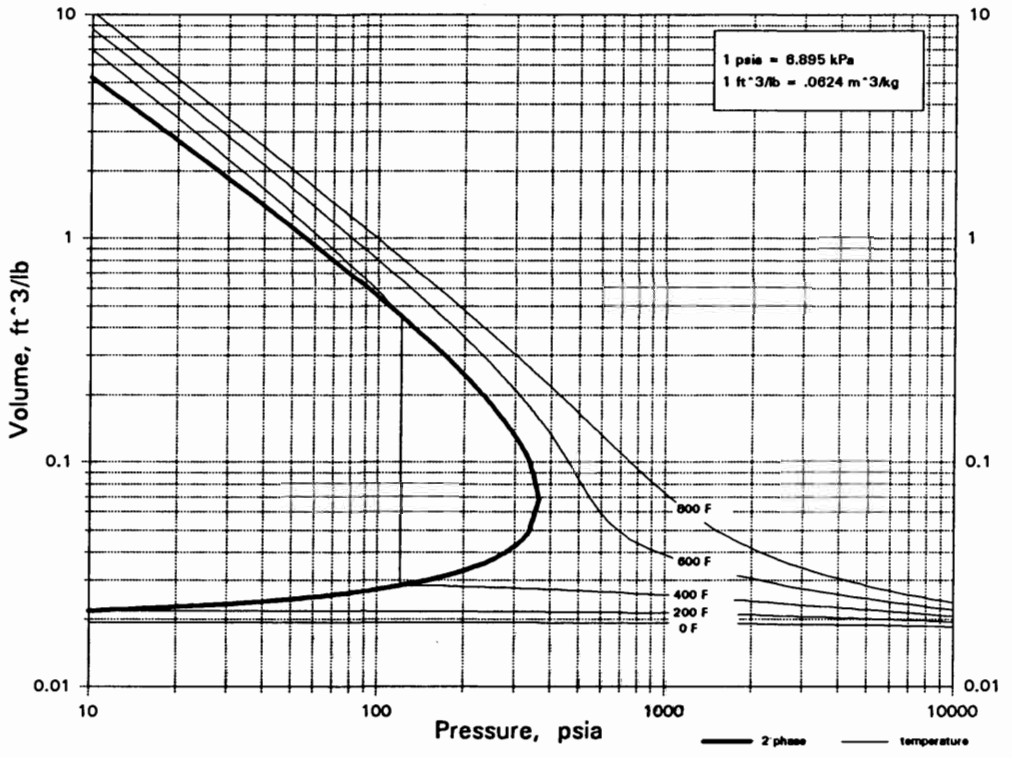


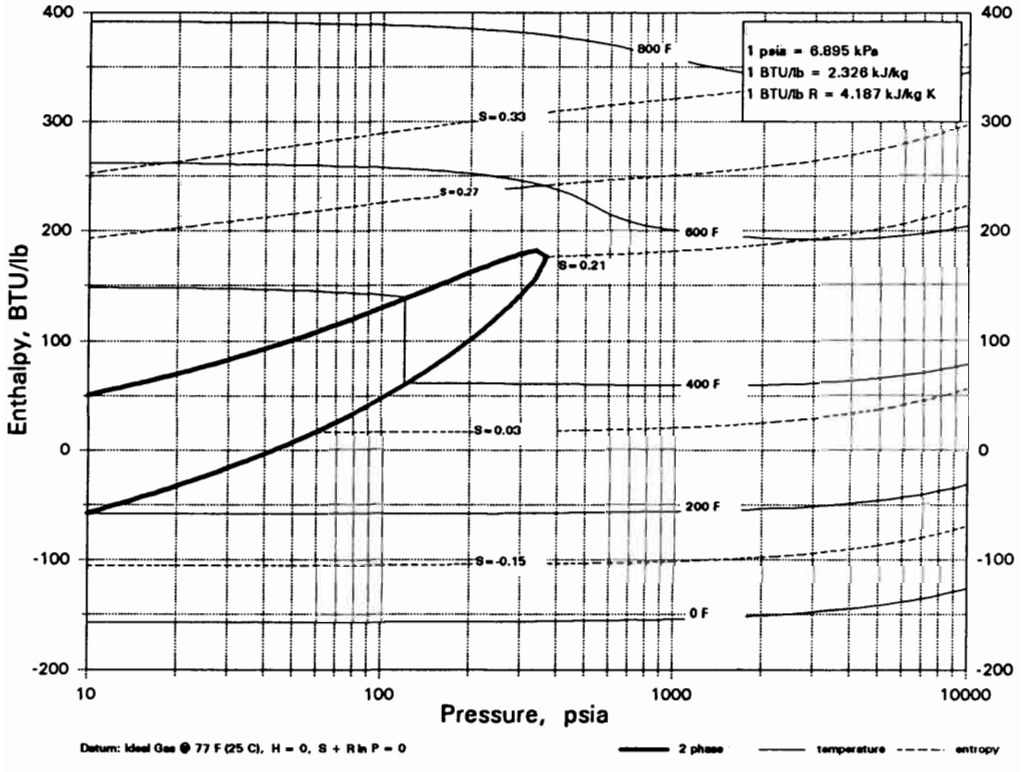
C8H18O Di-sec-BUTYL ETHER



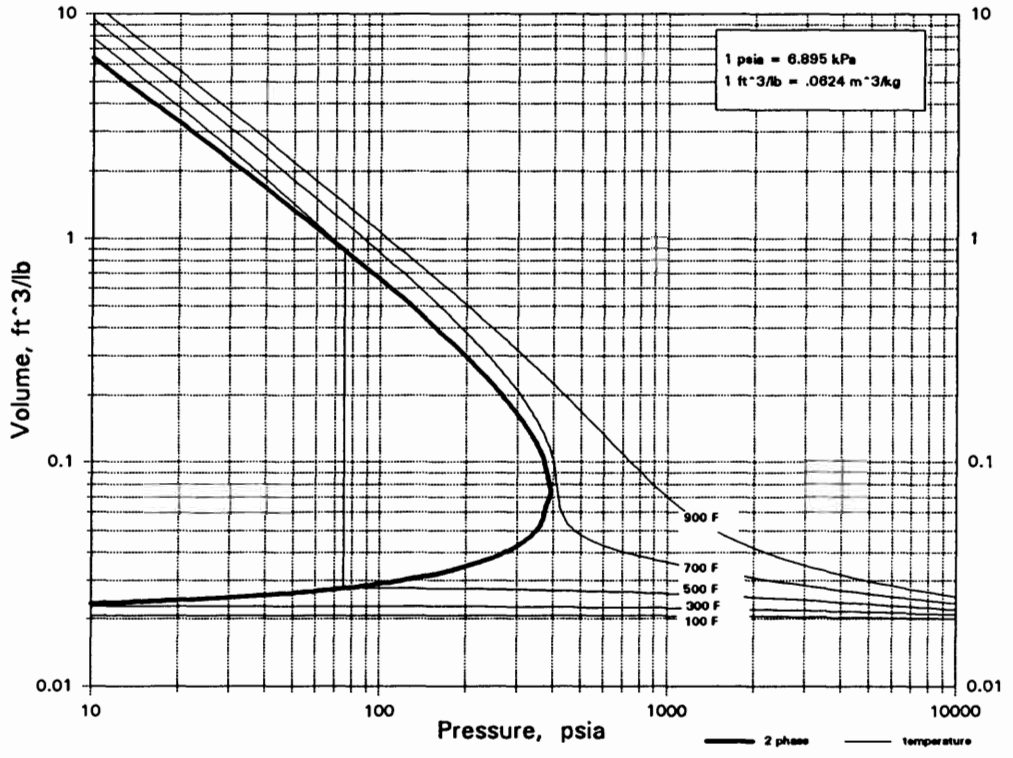


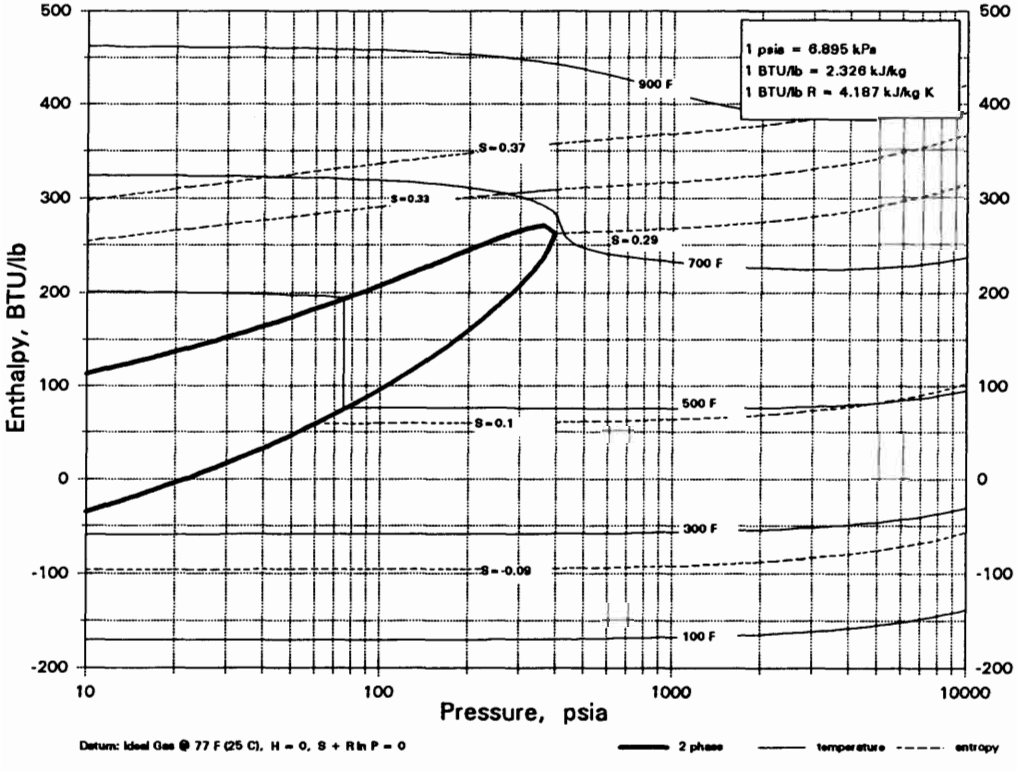
C8H18O DI-tert-BUTYL ETHER



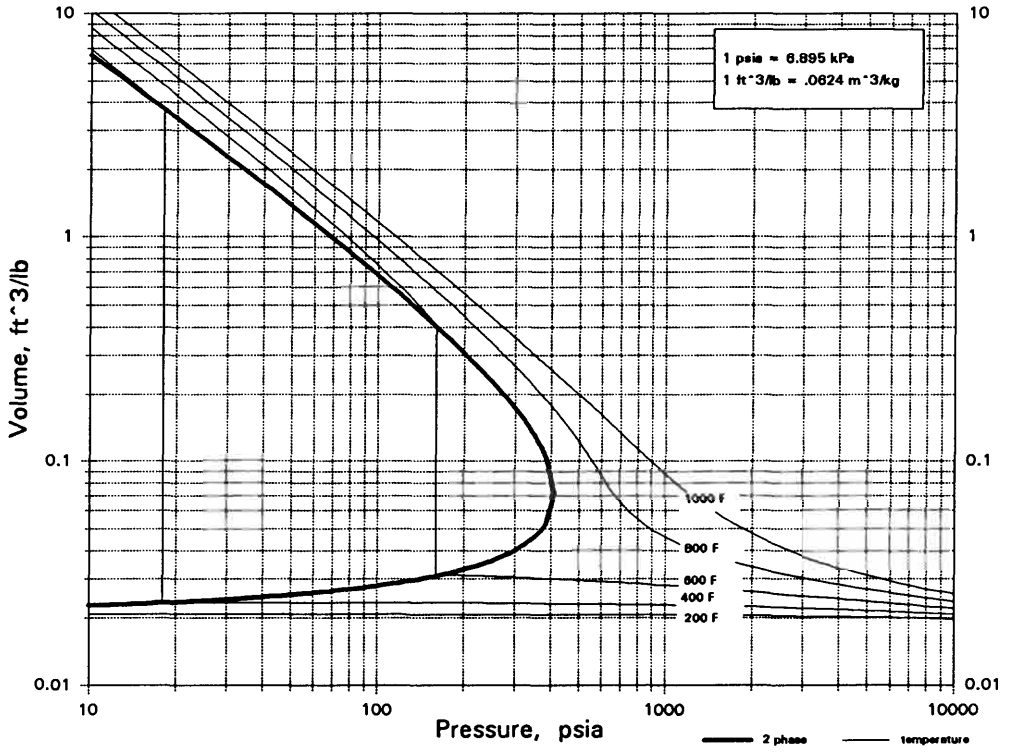


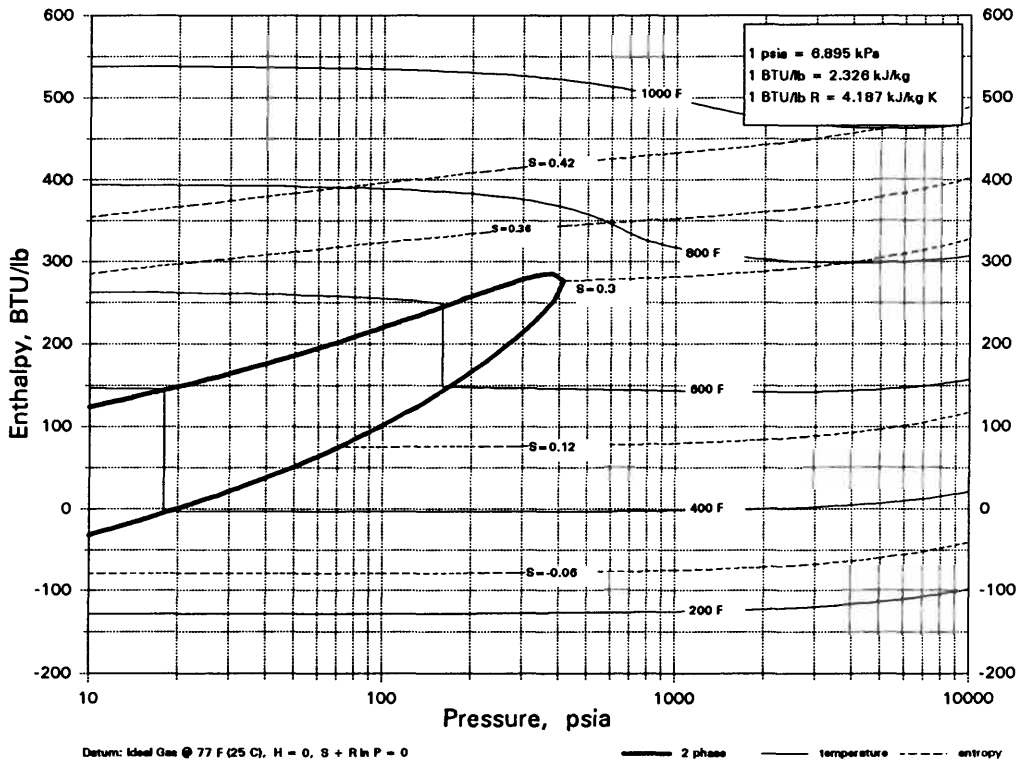
C8H18O 2-ETHYL-1-HEXANOL



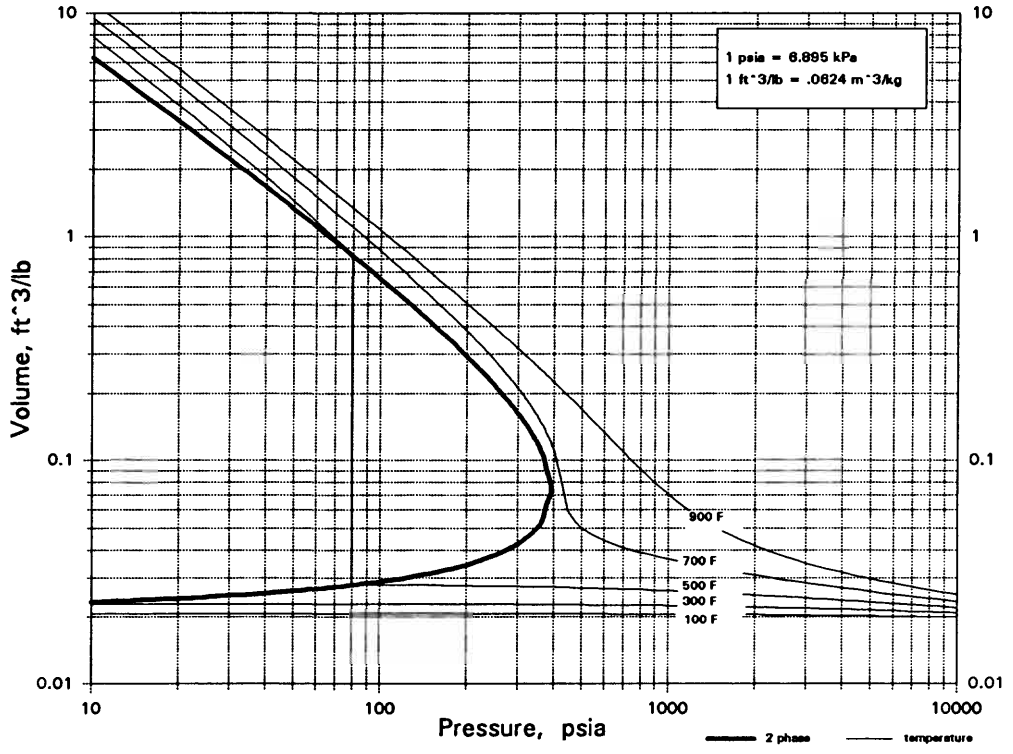


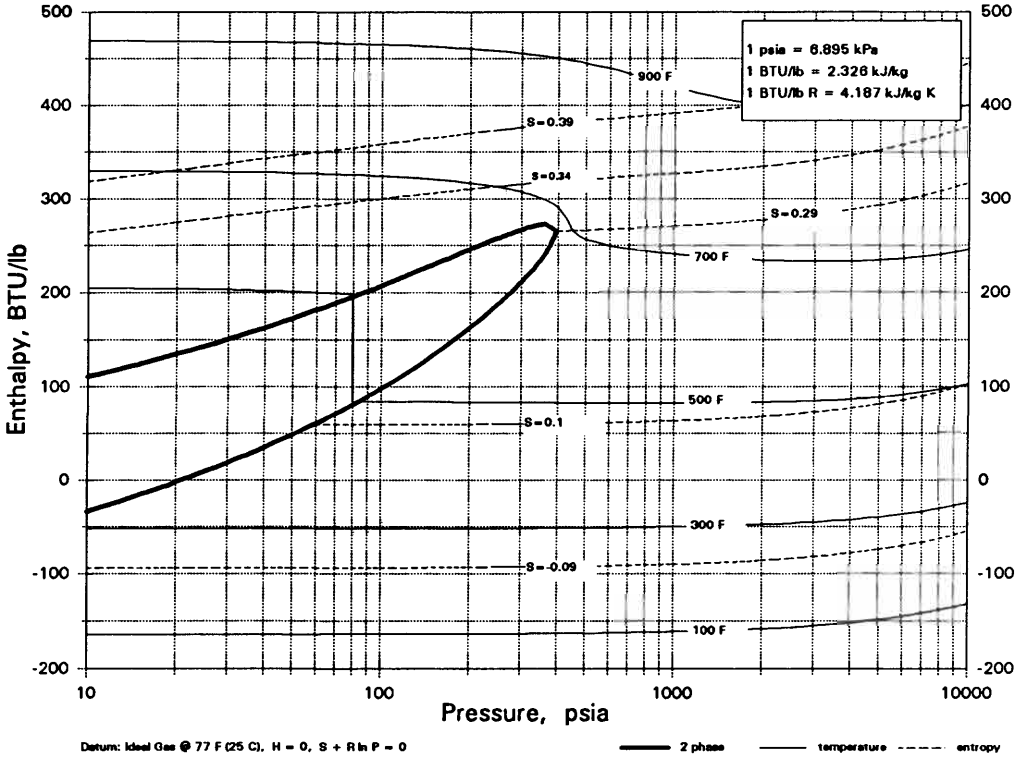
C8H18O 1-OCTANOL



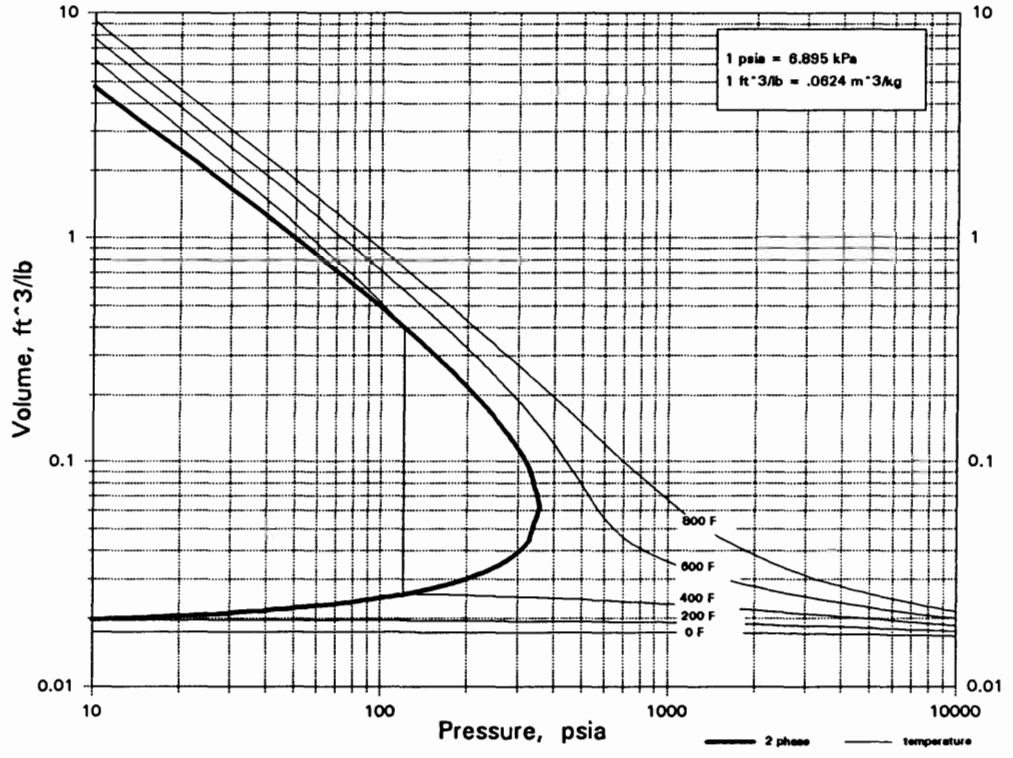


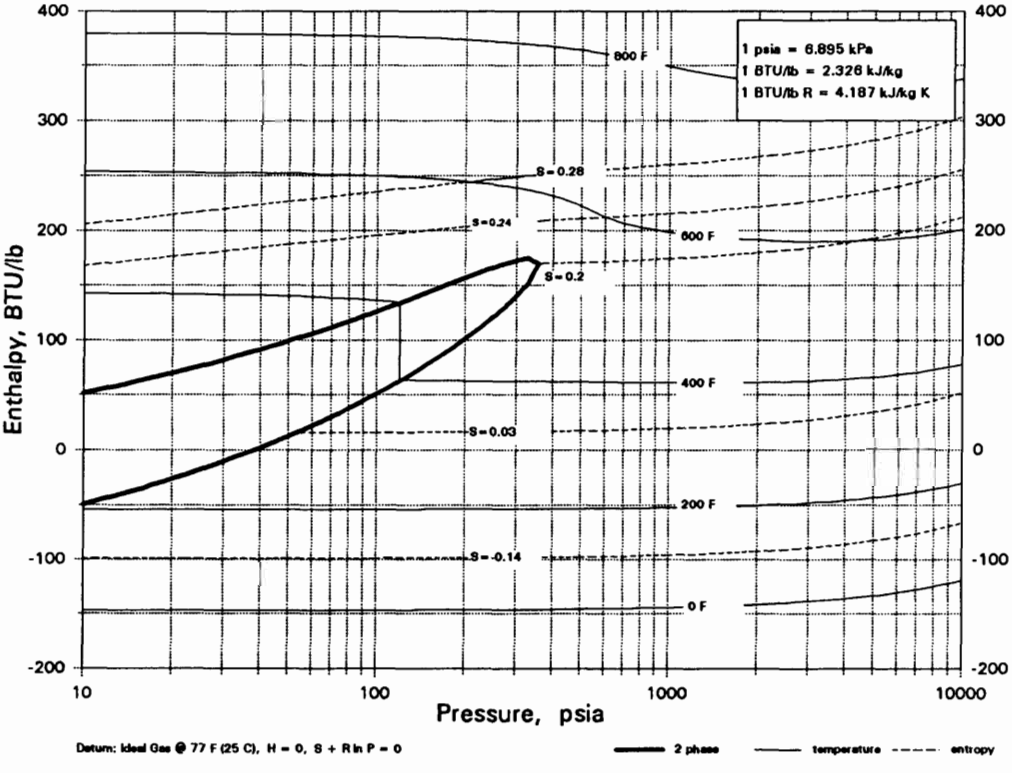
C8H18O 2-OCTANOL



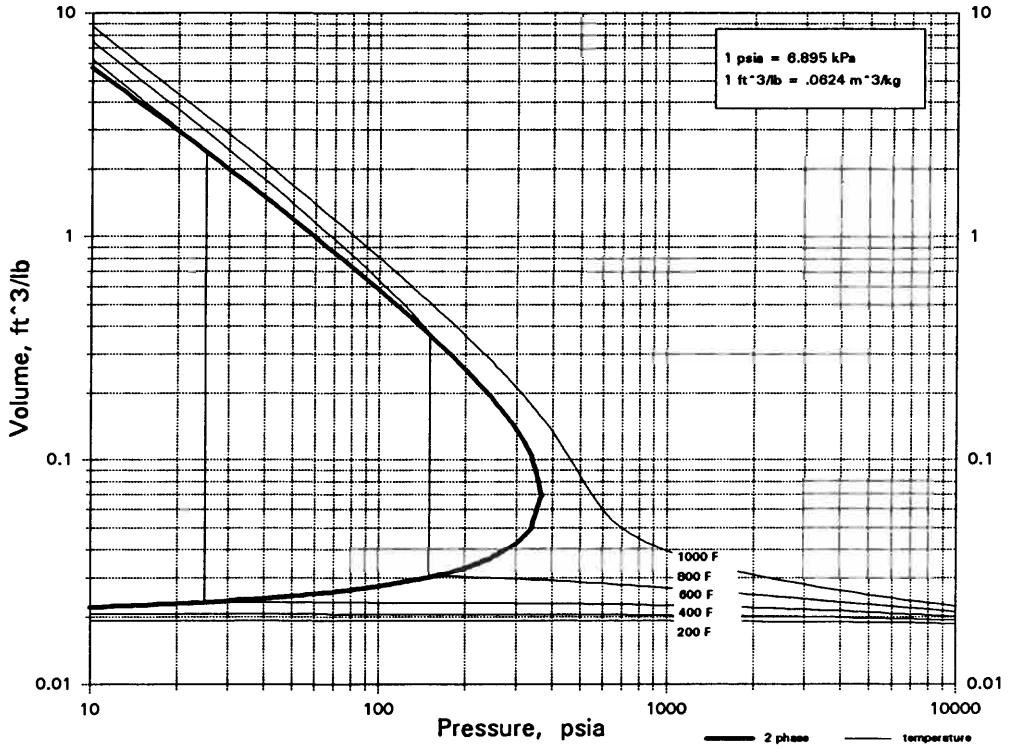


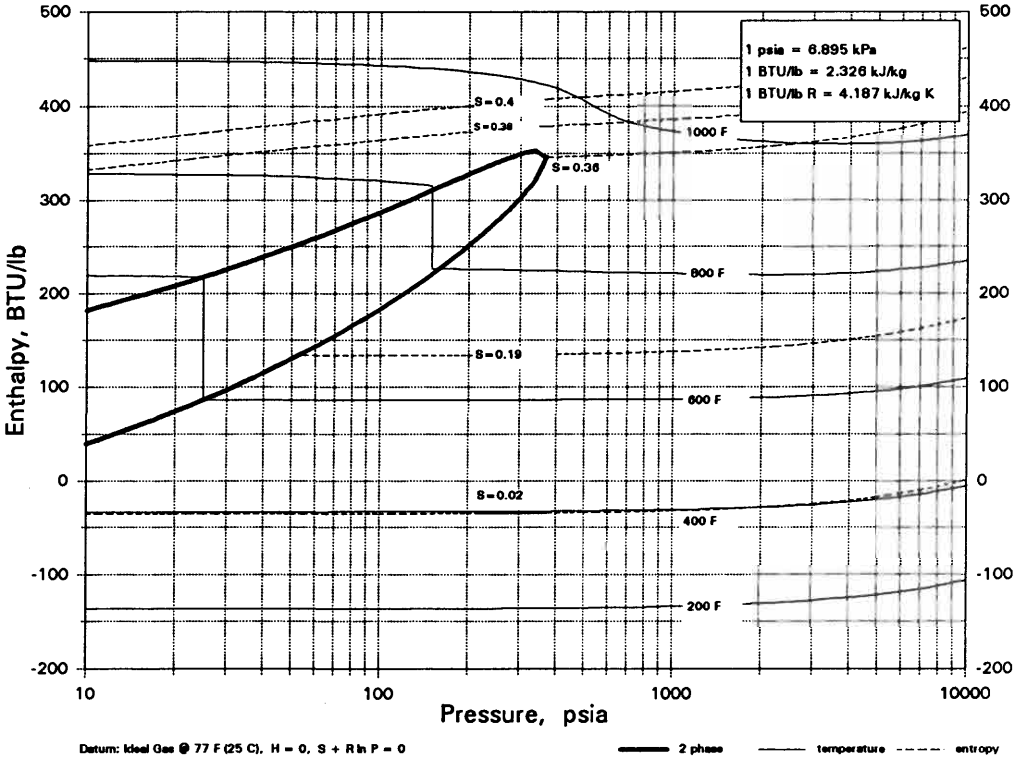
C8H18O2 DI-t-BUTYL PEROXIDE



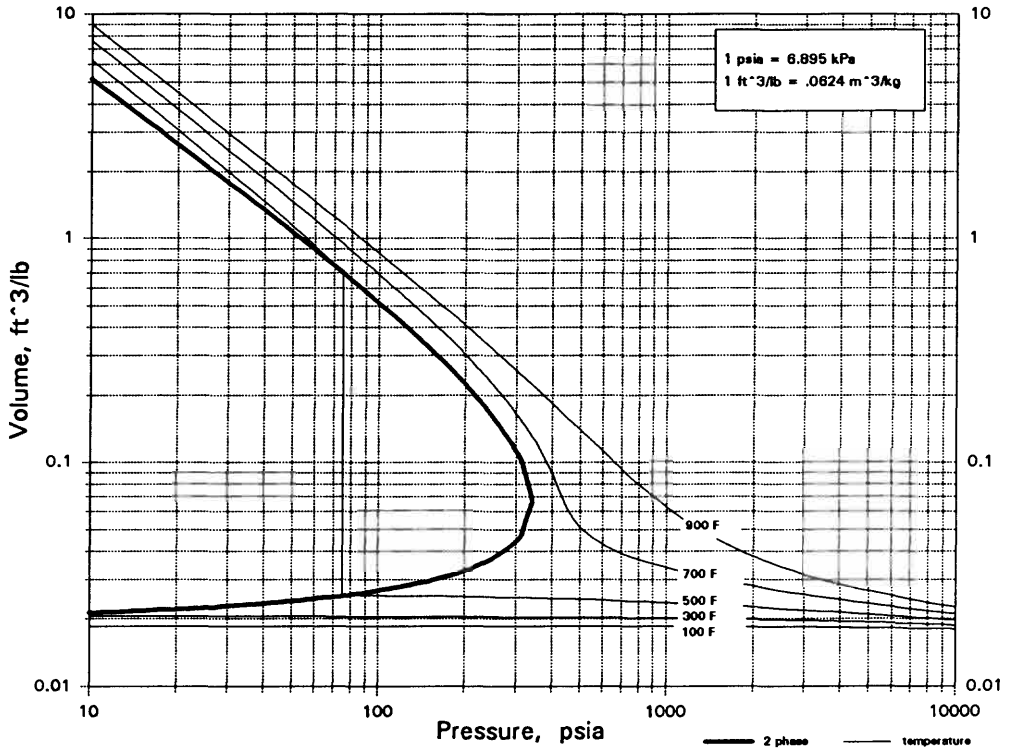


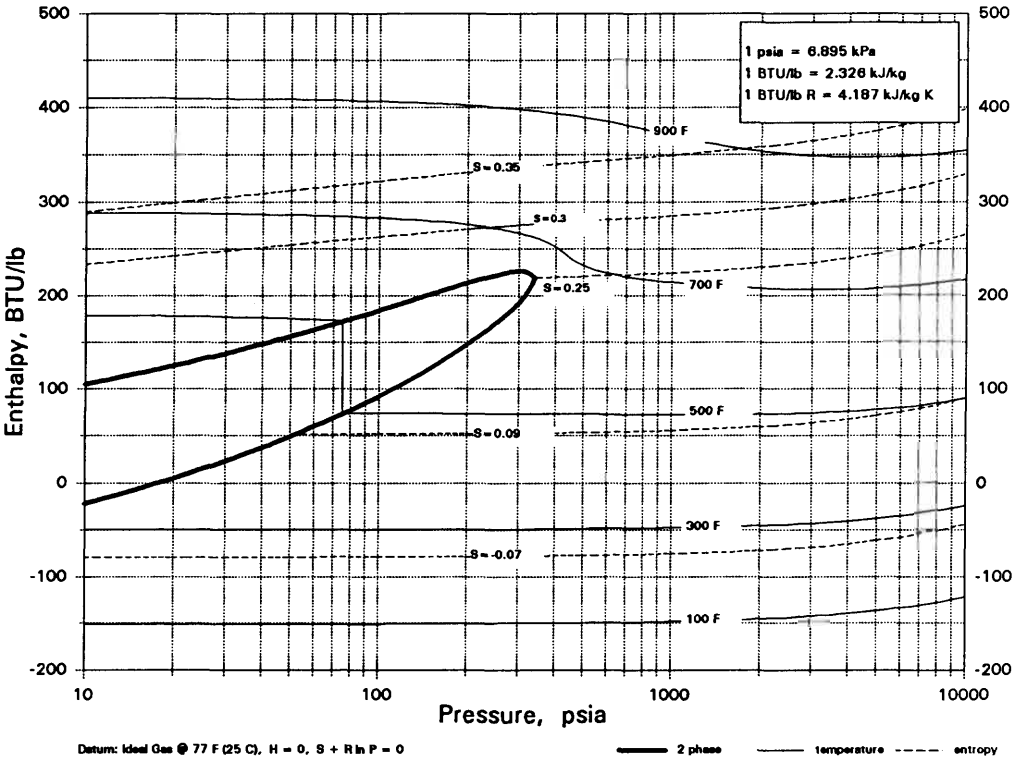
C8H18O2S DI-n-BUTYL SULFONE



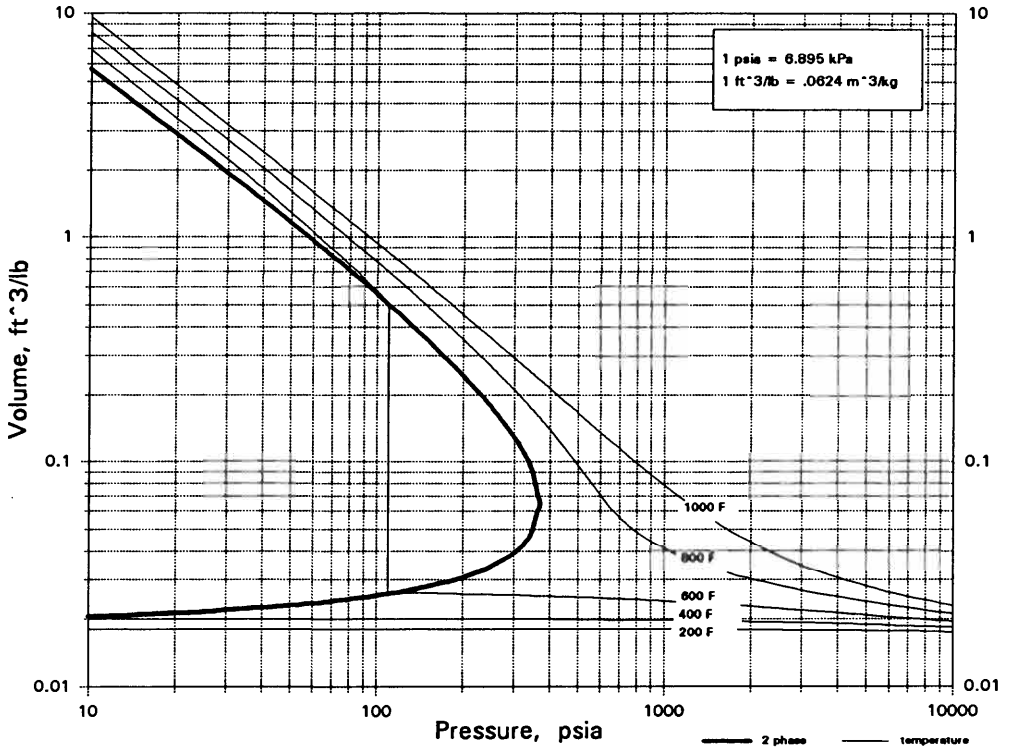


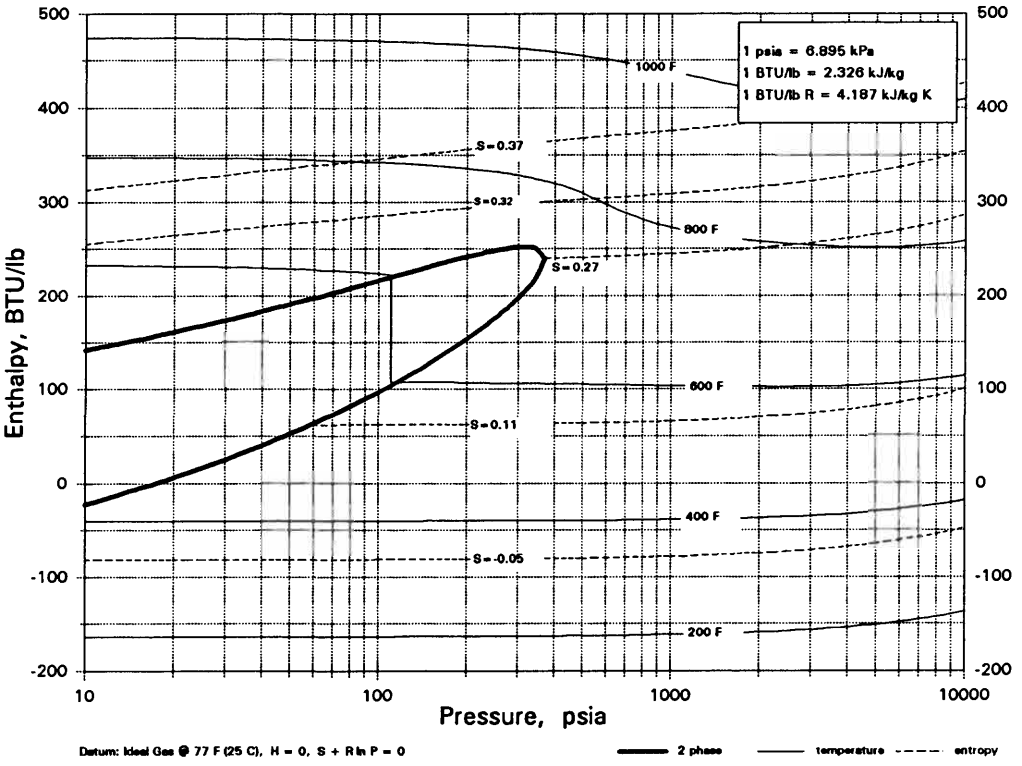
C8H18O3 DIETHYLENE GLYCOL DIETHYL ETHER



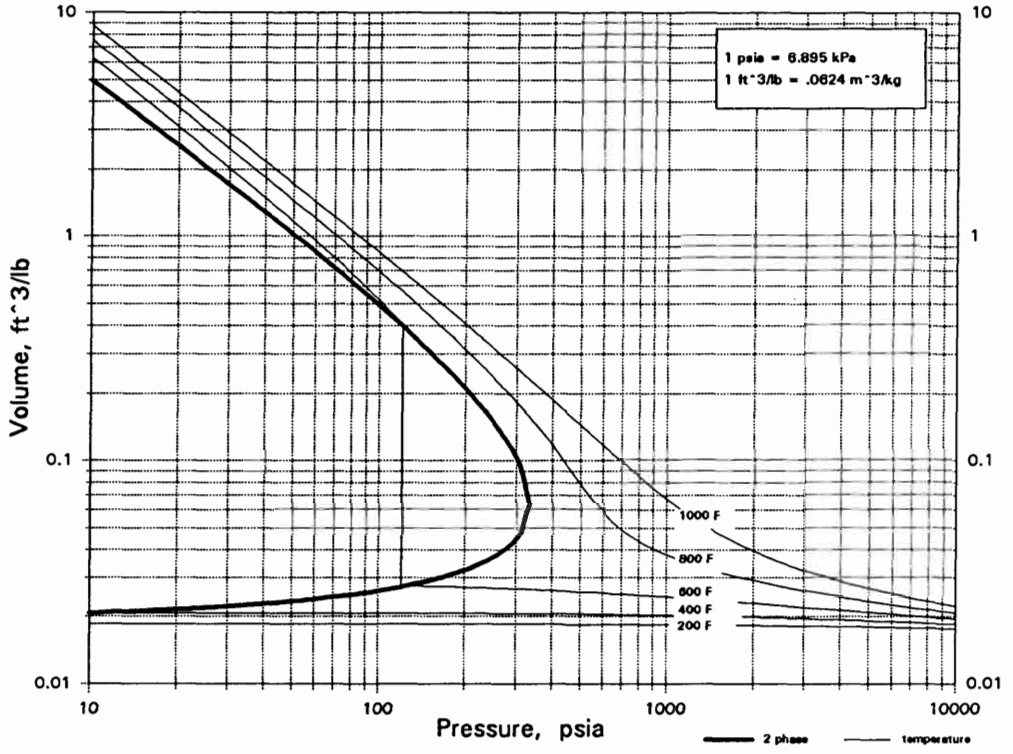


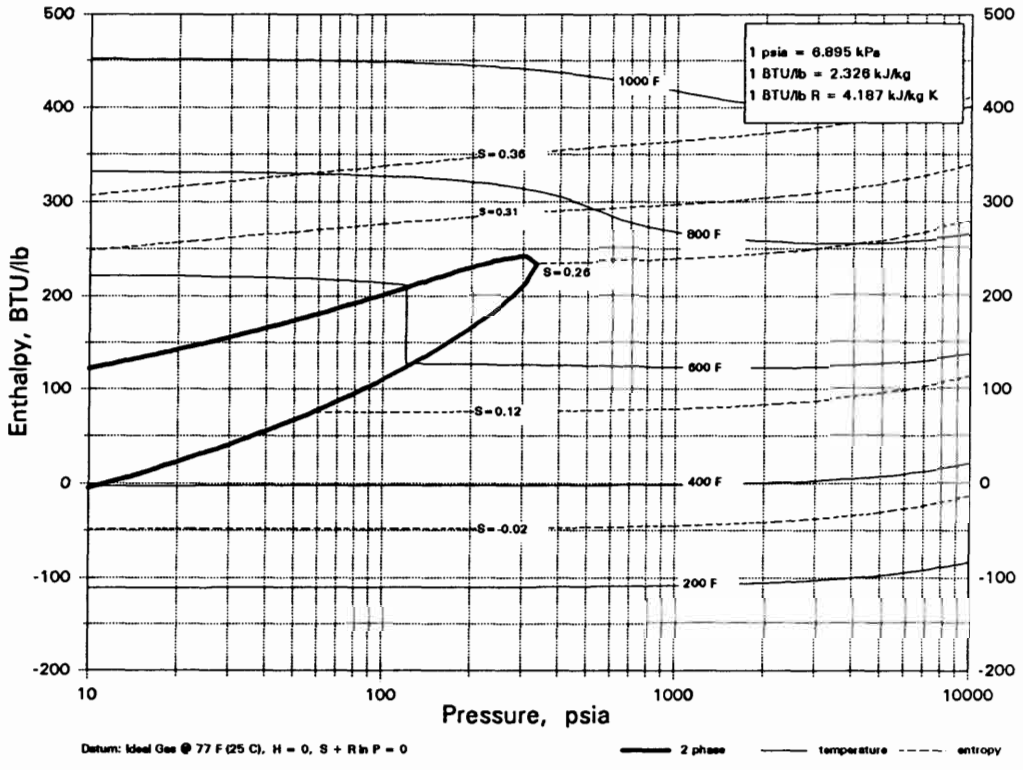
C8H18O3 DIETHYLENE GLYCOL MONOBUTYL ETHER



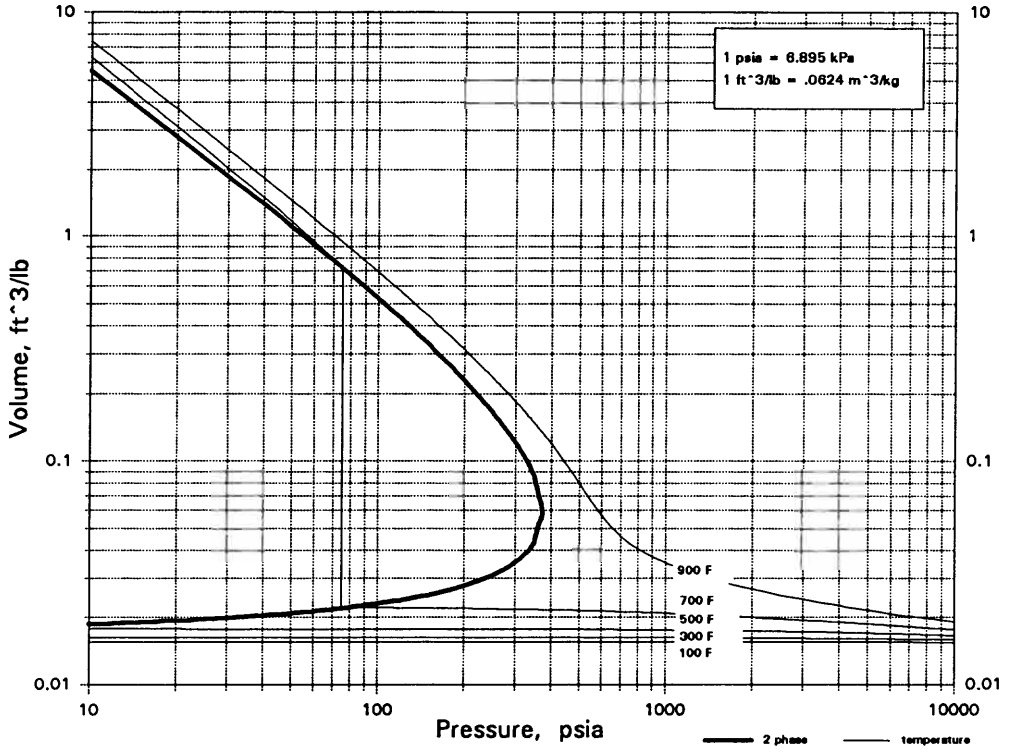


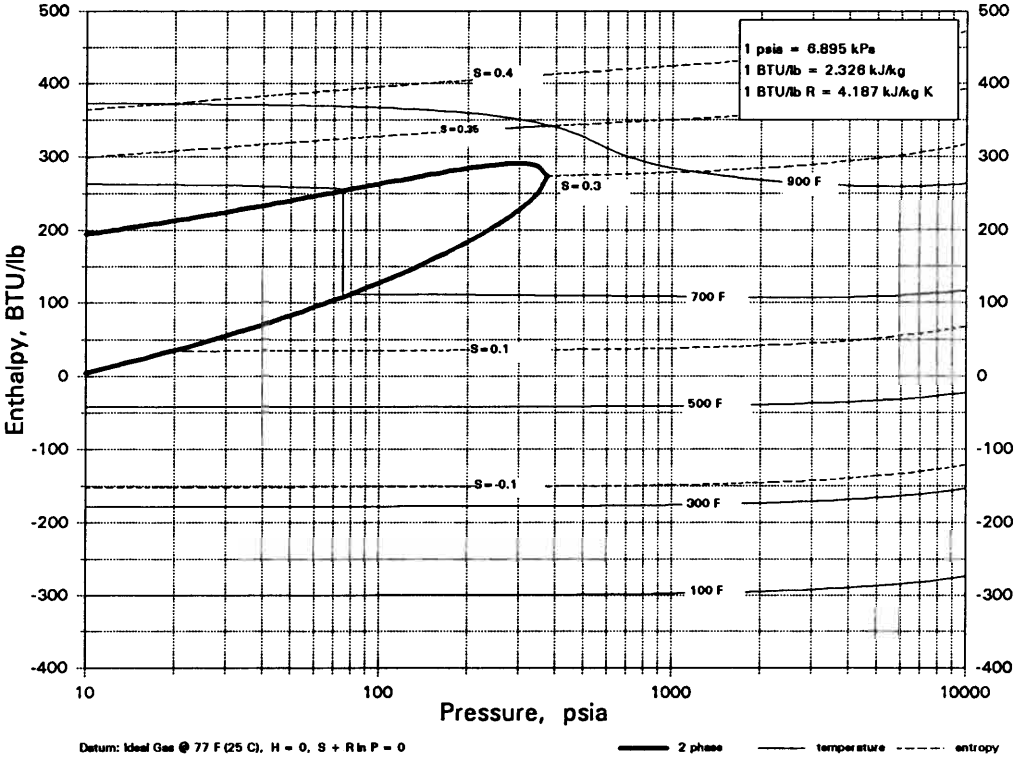
C8H18O4 TRIETHYLENE GLYCOL DIMETHYL ETHER



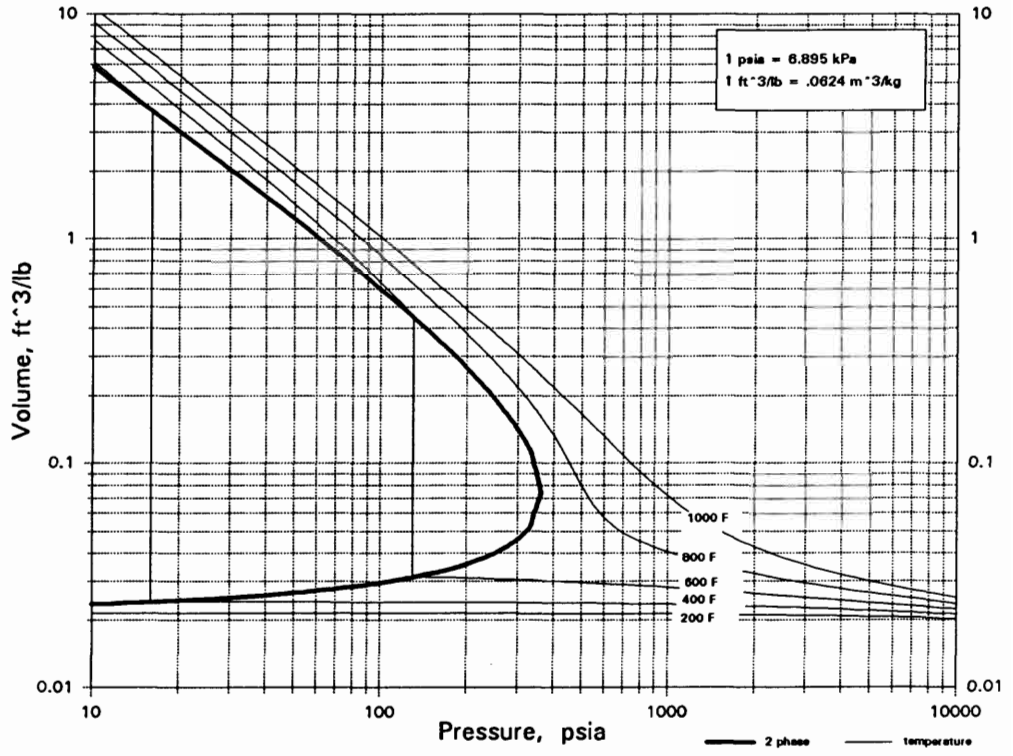


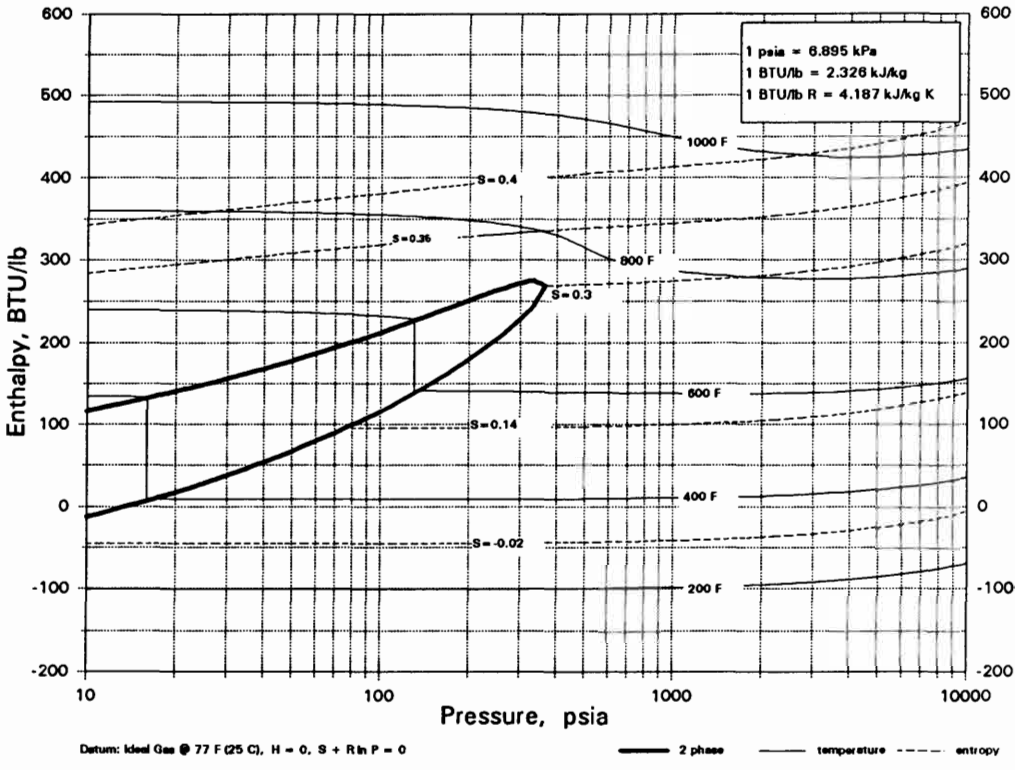
C8H18O5 TETRAETHYLENE GLYCOL



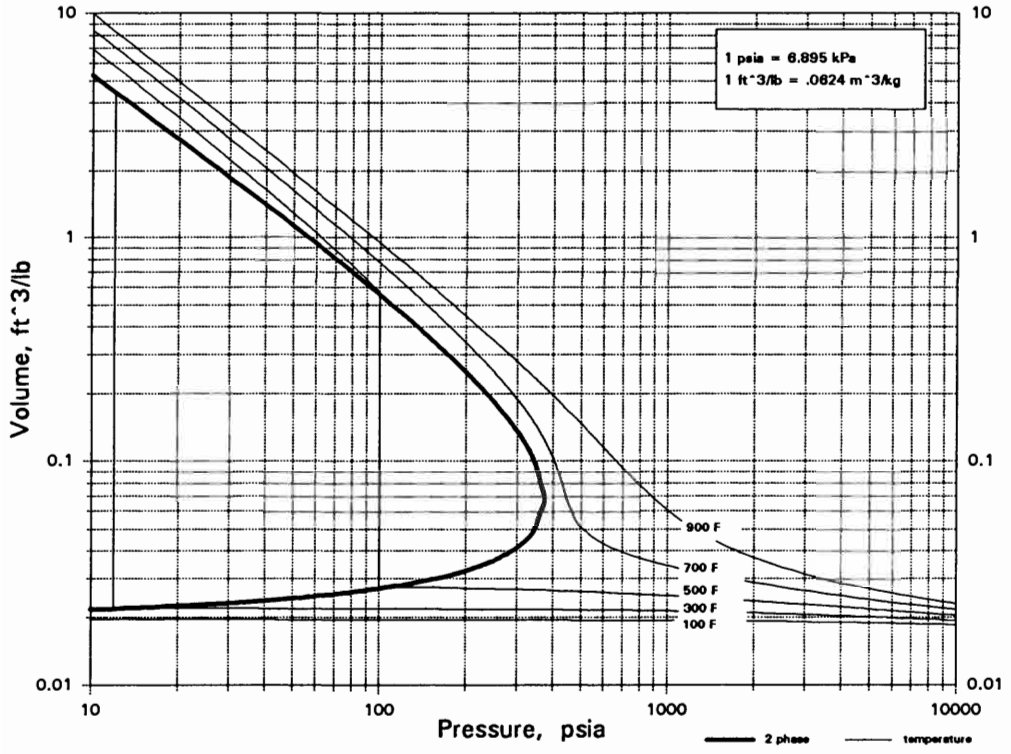


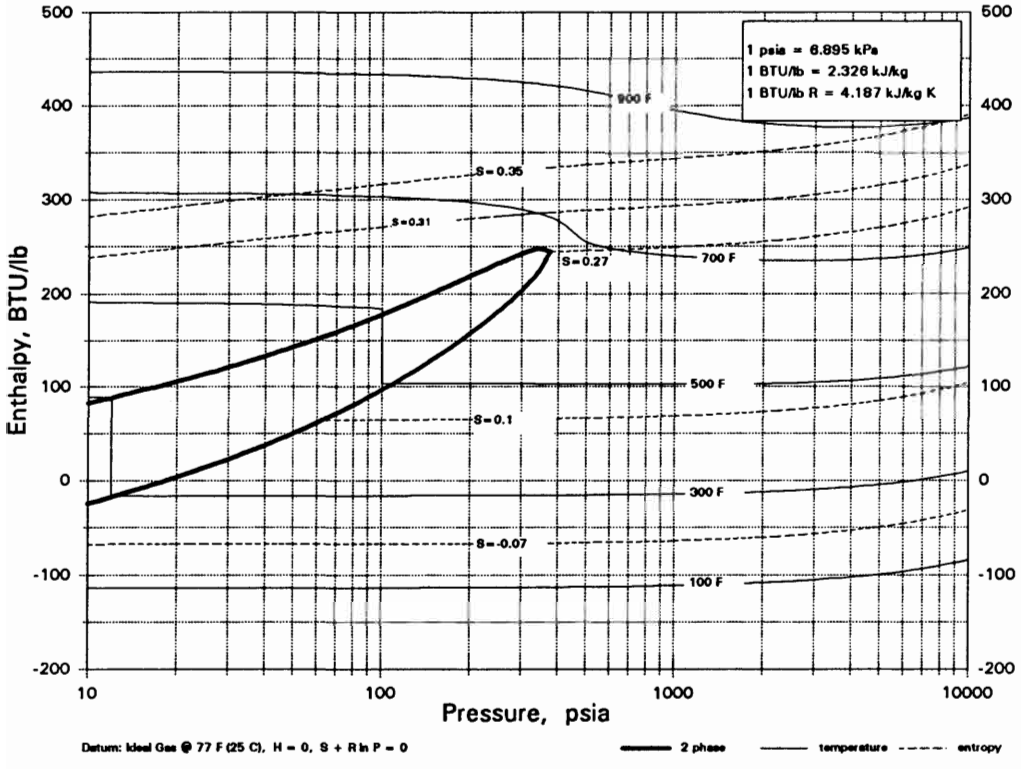
C8H18S n-OCTYL MERCAPTAN



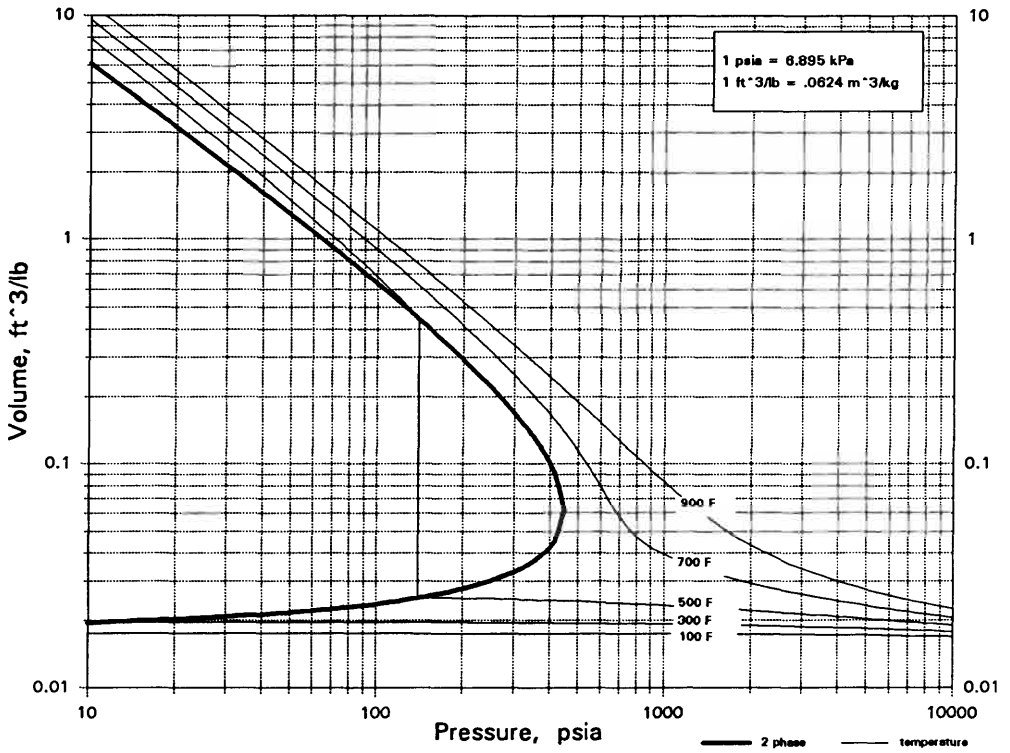


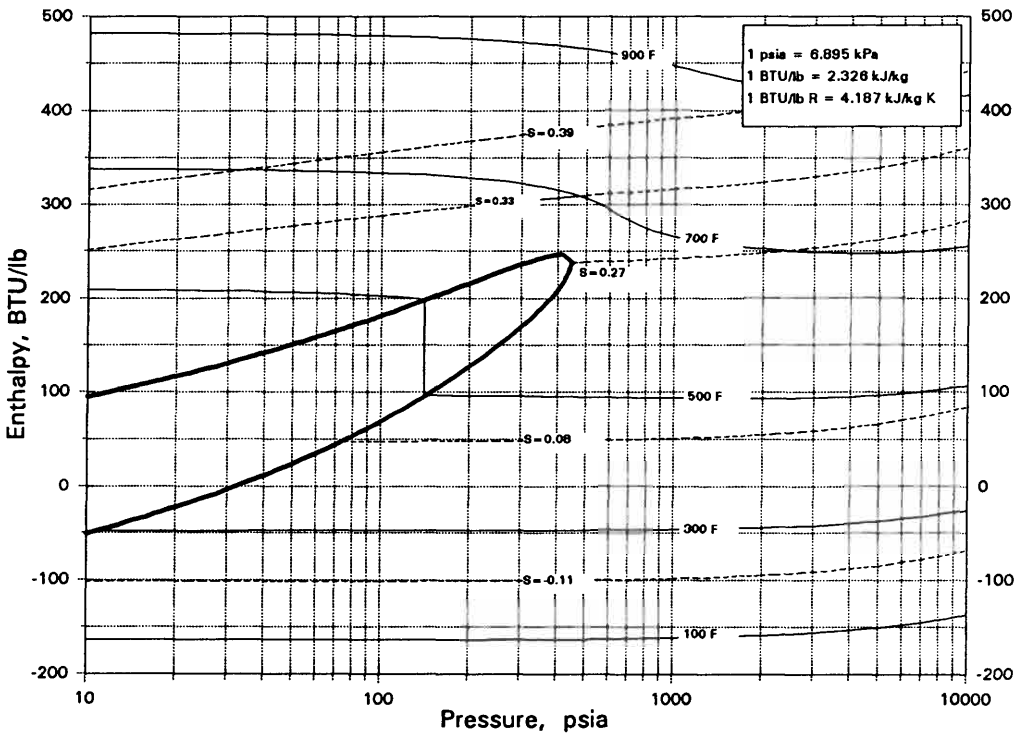
C8H18S tert-OCTYL MERCAPTAN



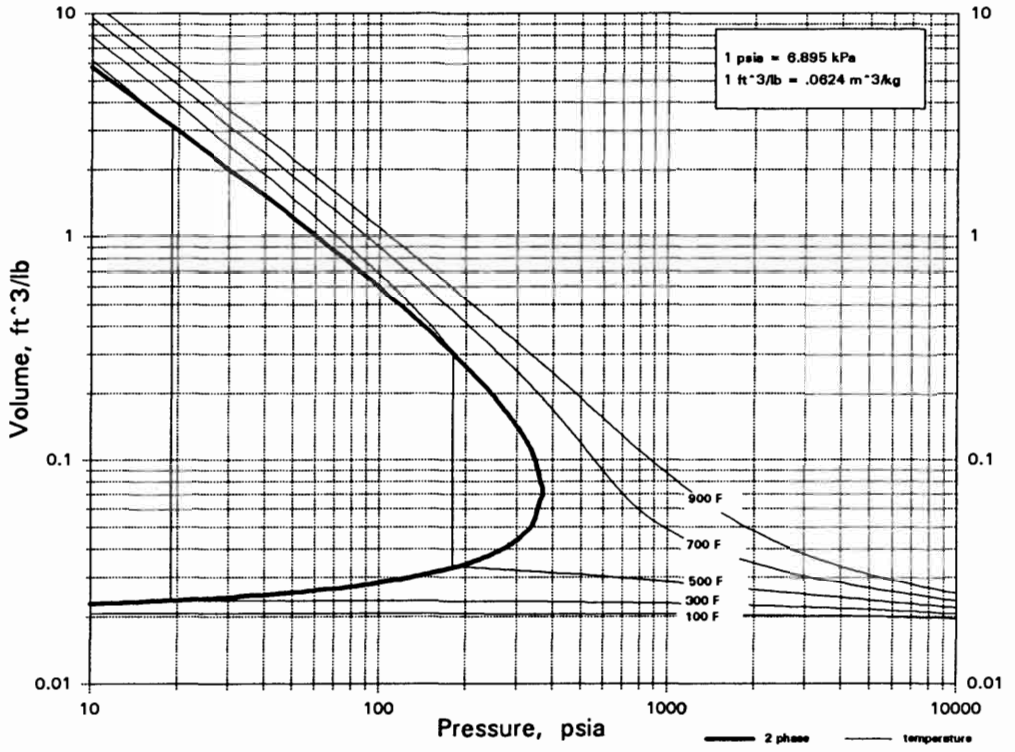


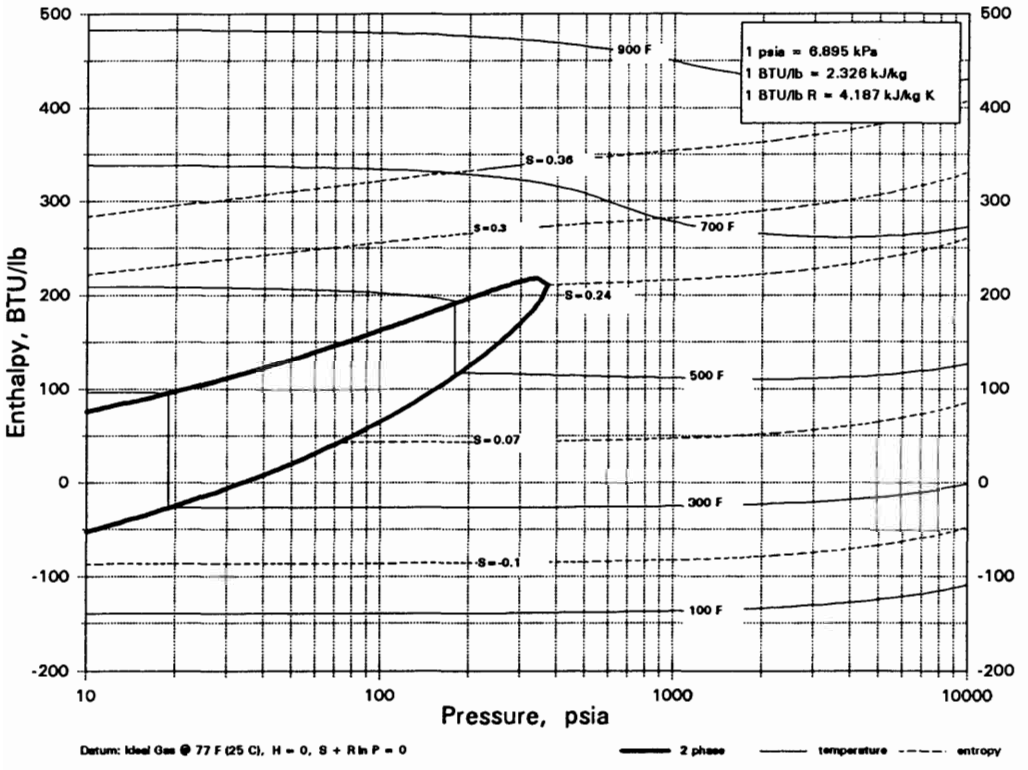
C8H19N DI-n-BUTYLAMINE



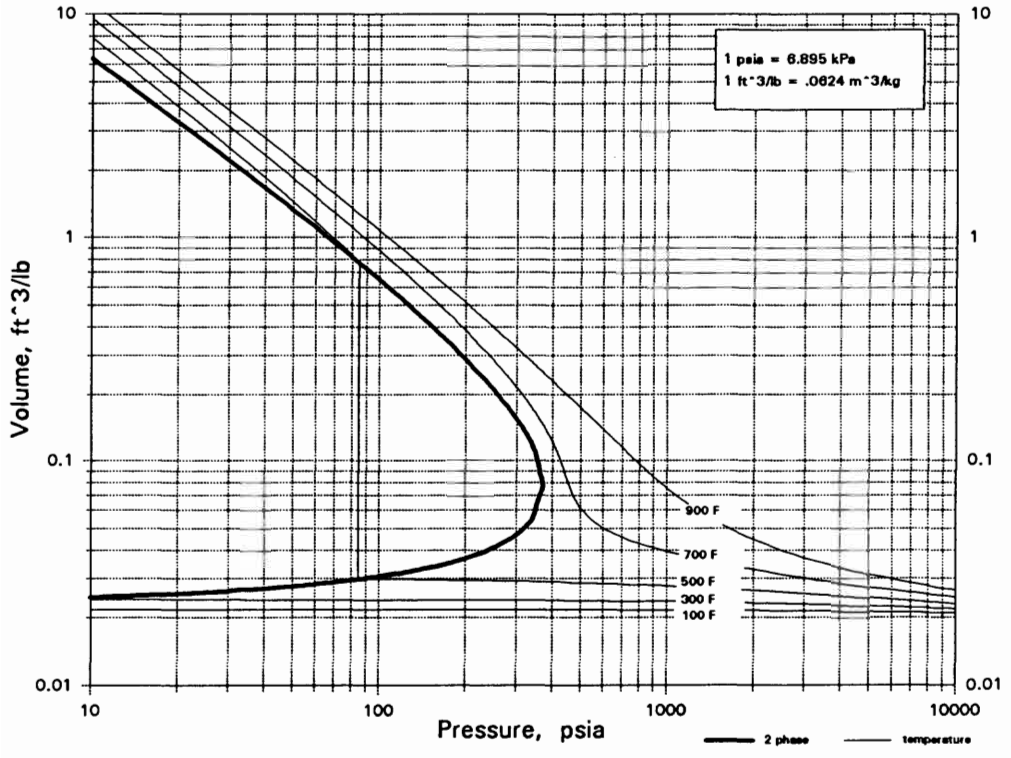


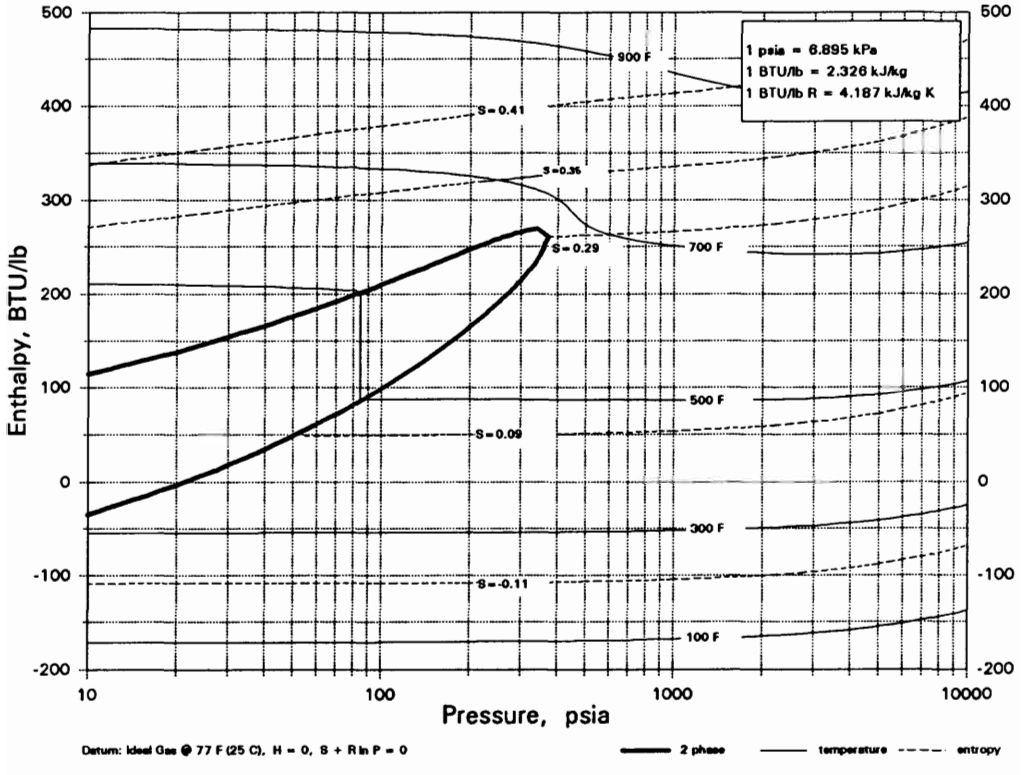
C8H19N DIISOBUTYLAMINE



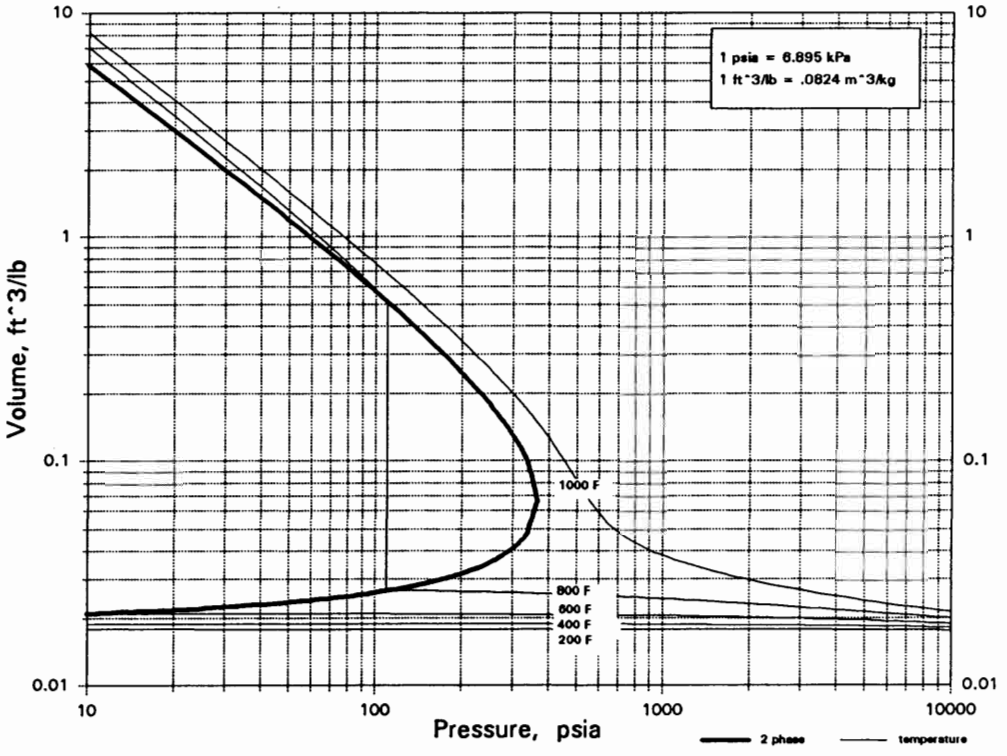


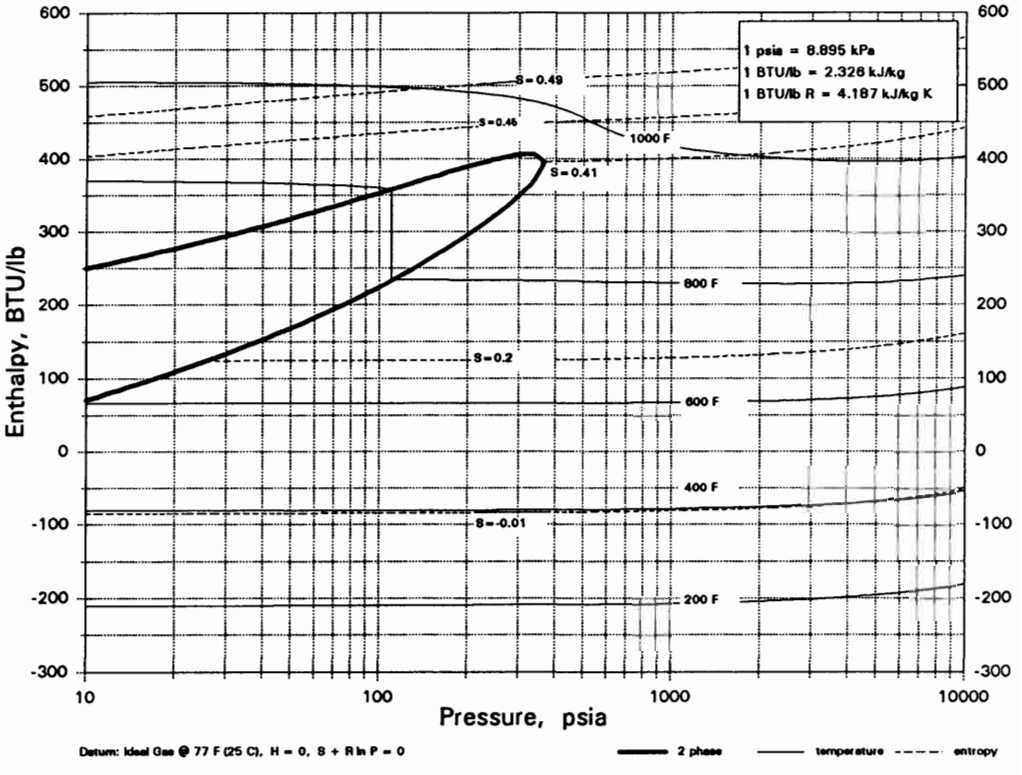
C8H19N n-OCTYLAMINE



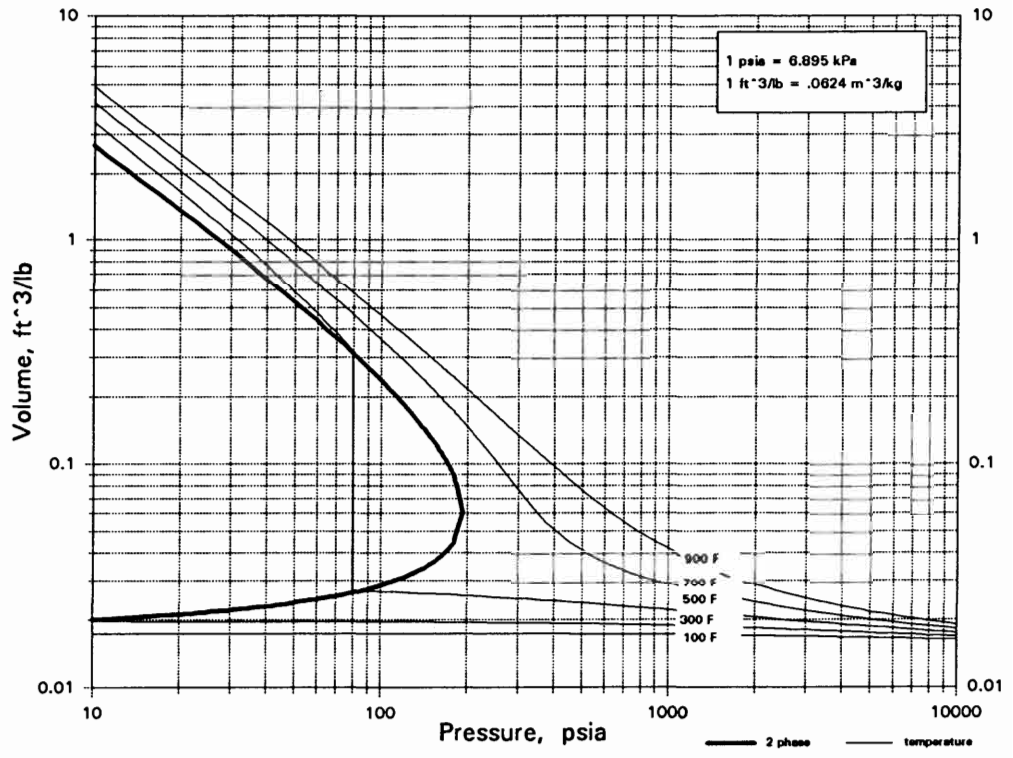


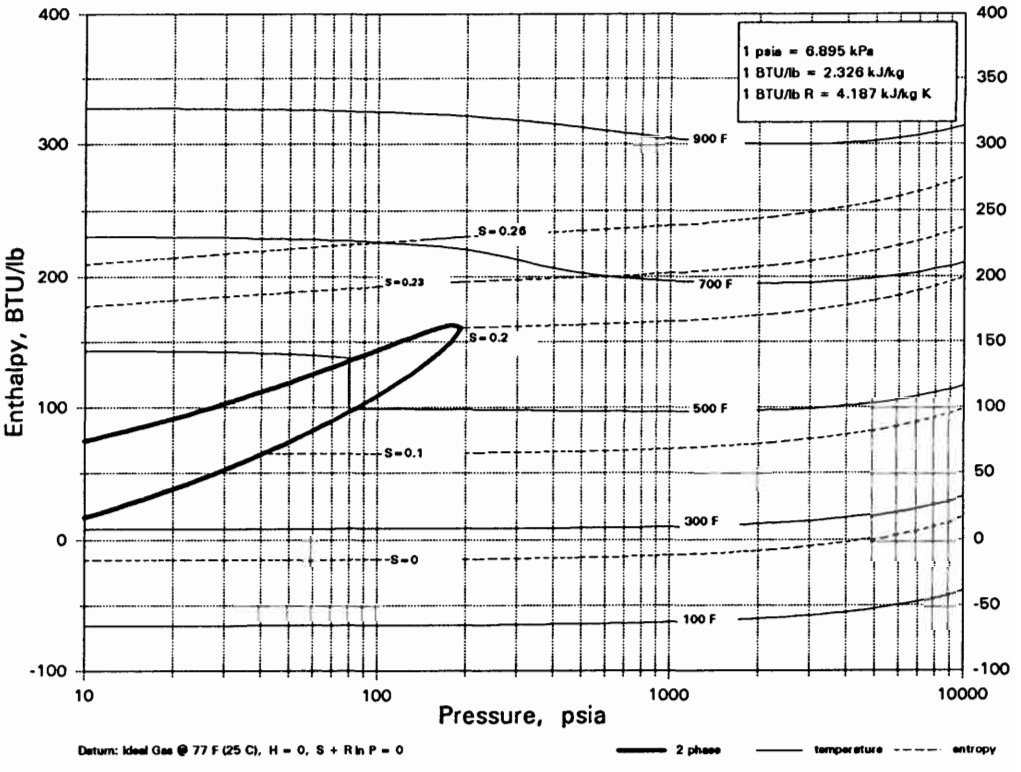
C8H23N5 TETRAETHYLENEPENTAMINE



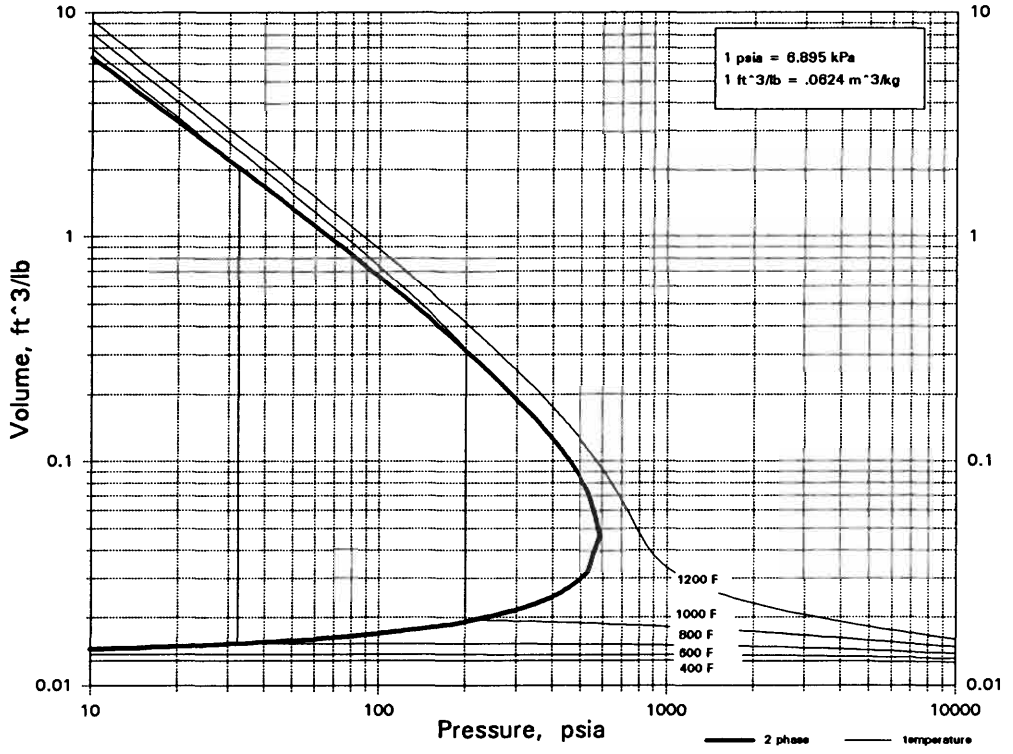


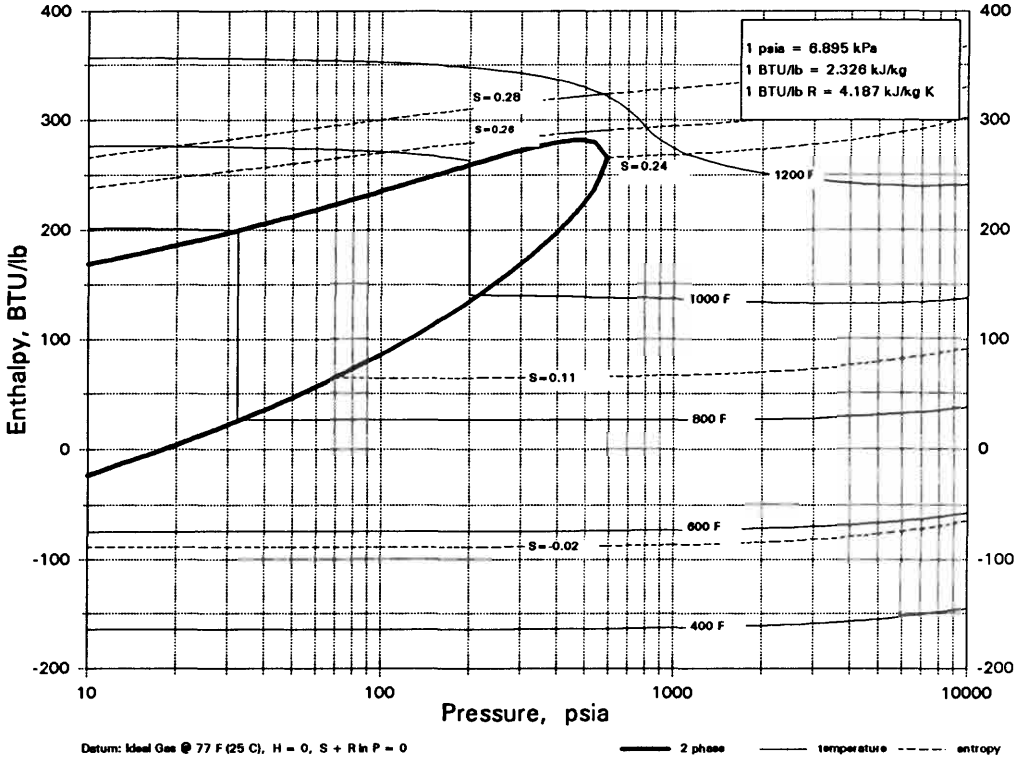
C8H24O4Si4 OCTAMETHYLCYCLOTETRASILOXANE



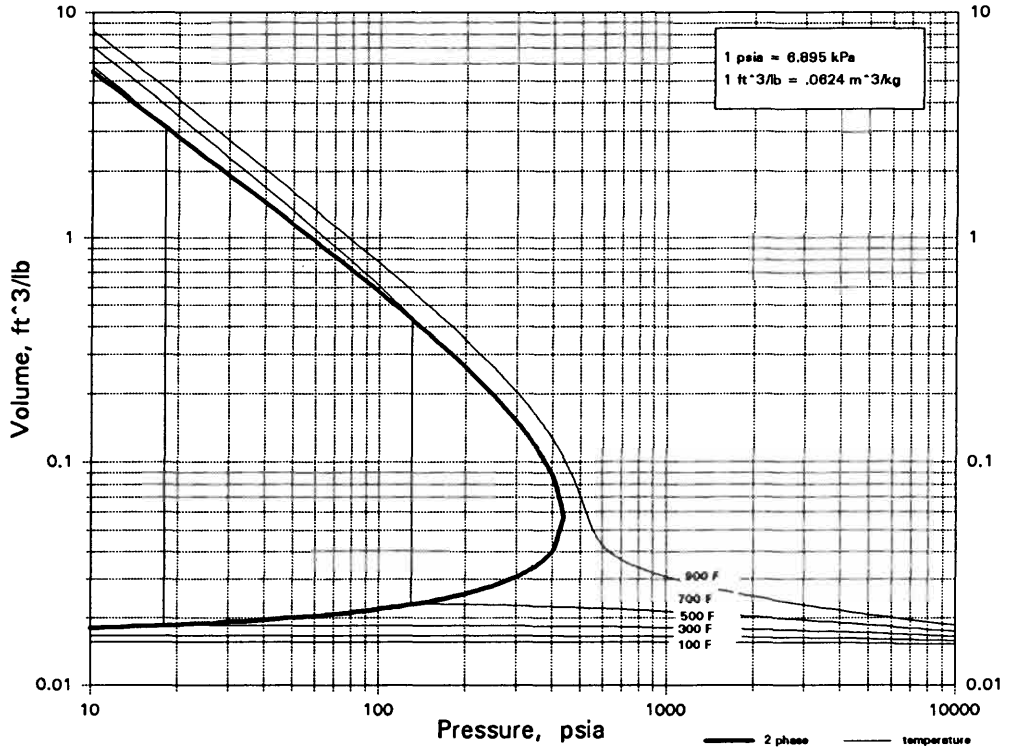


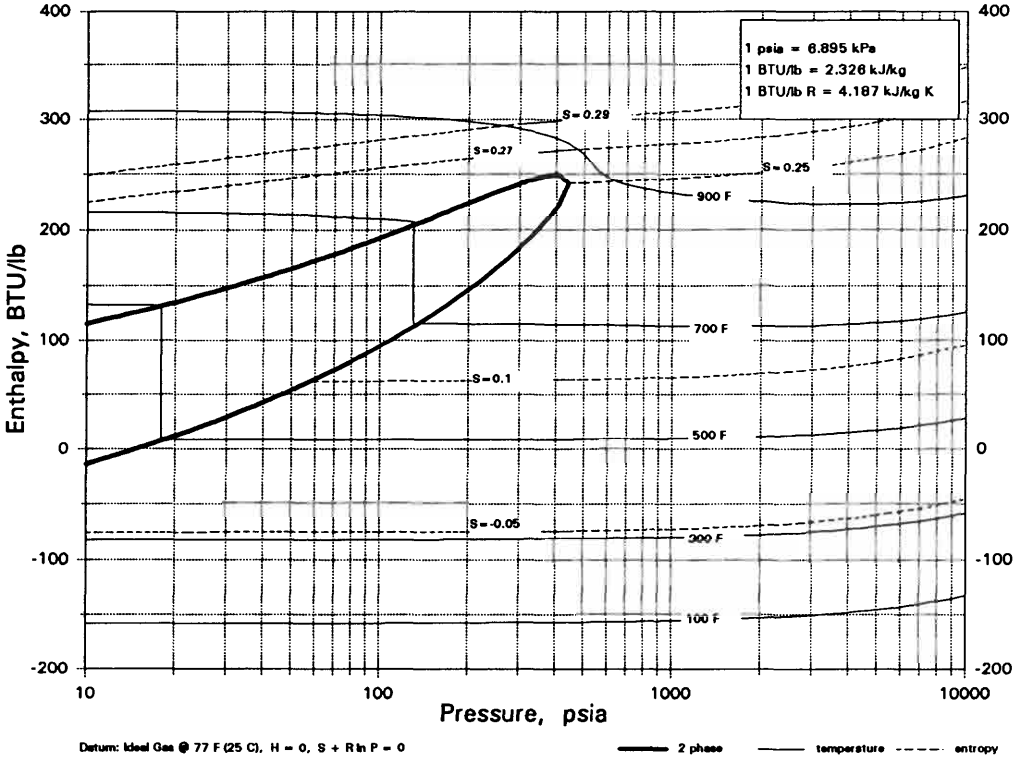
C9H4O5 TRIMELLITIC ANHYDRIDE



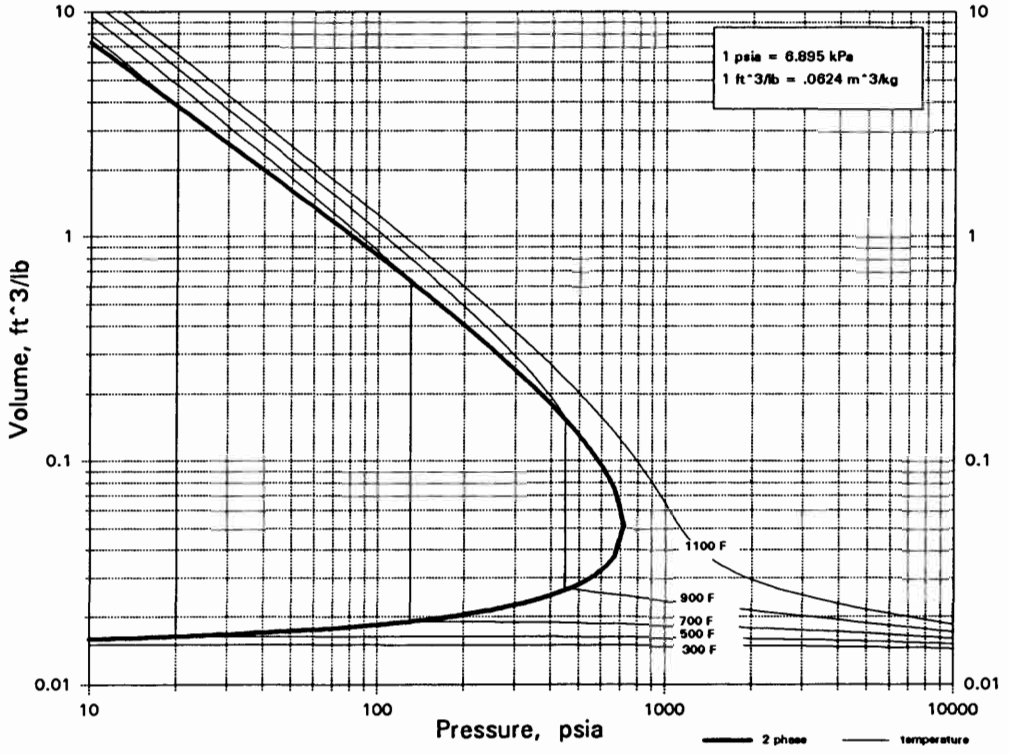


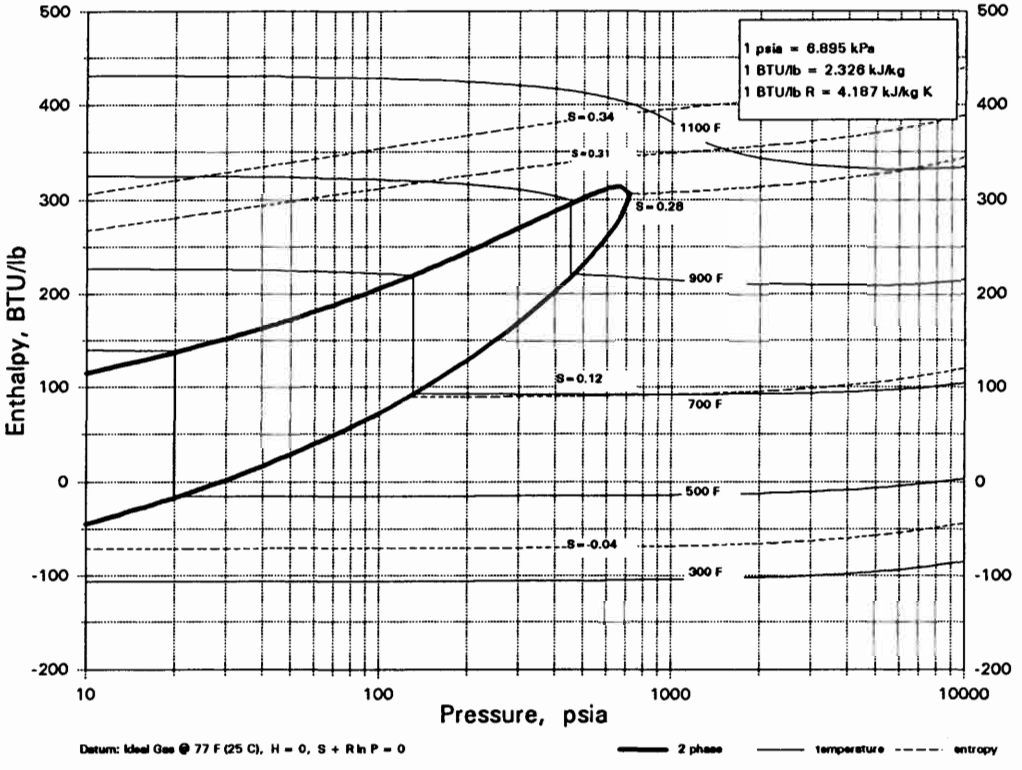
C9H6N2O2 TOLUENE DIISOCYANATE



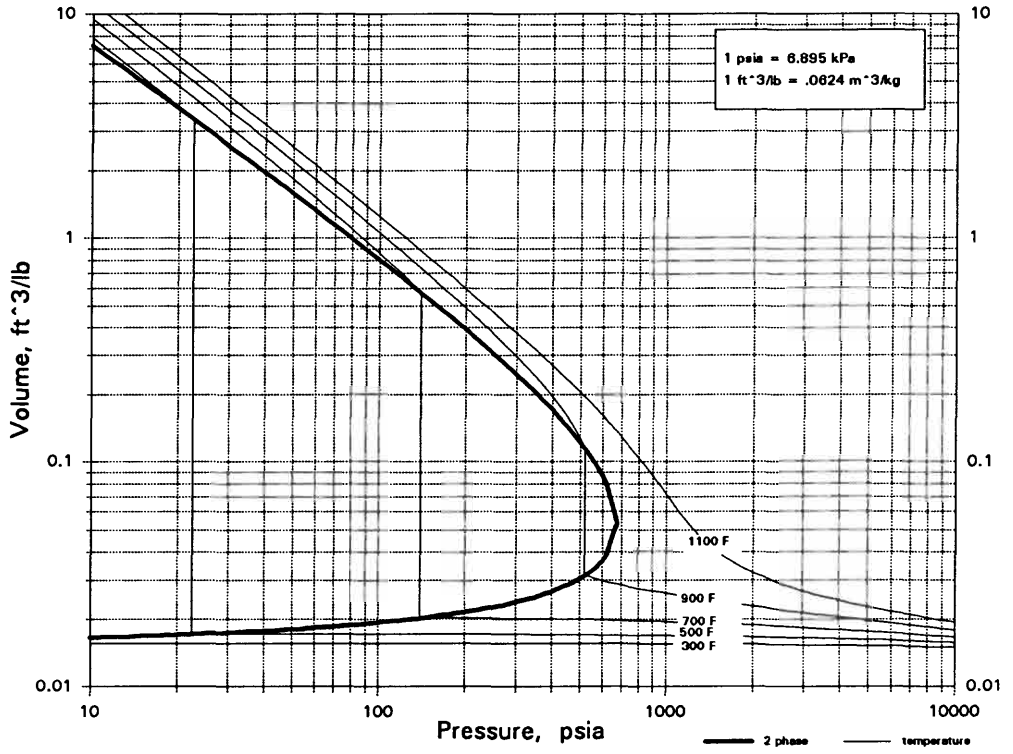


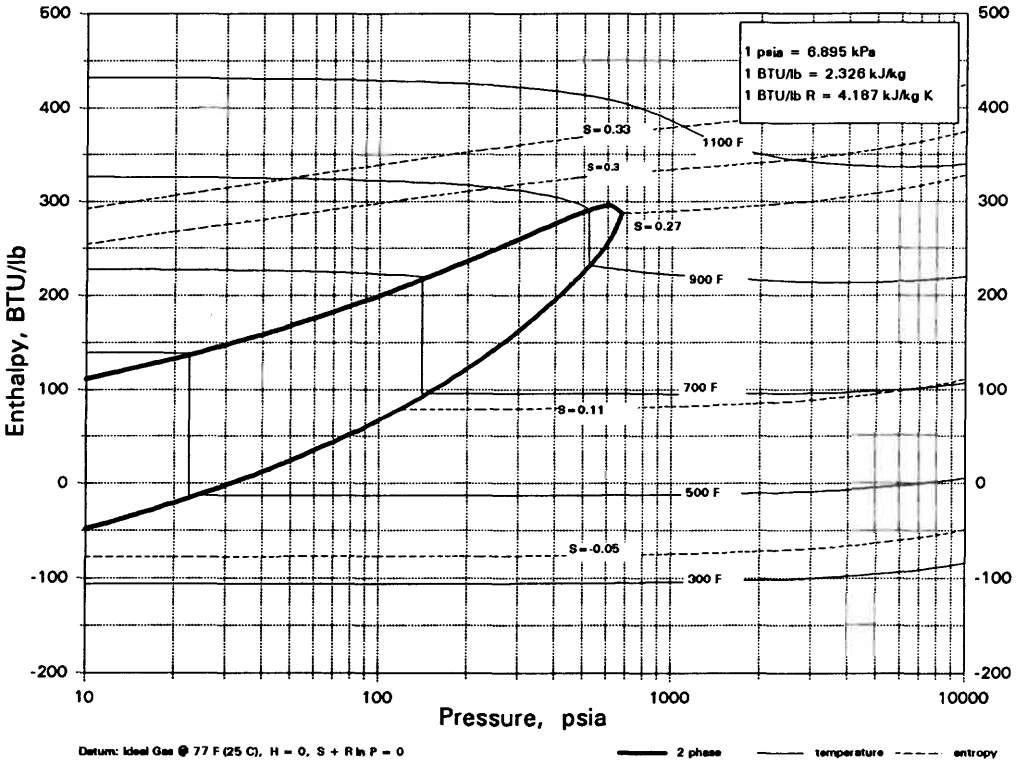
C9H7N ISOQUINOLINE



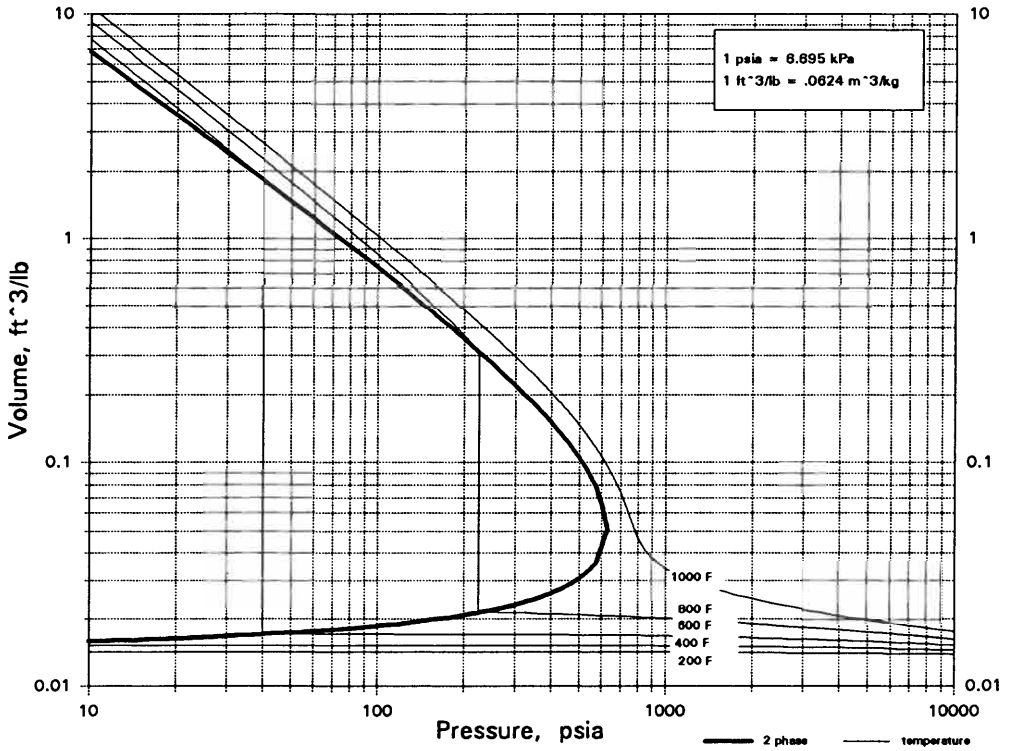


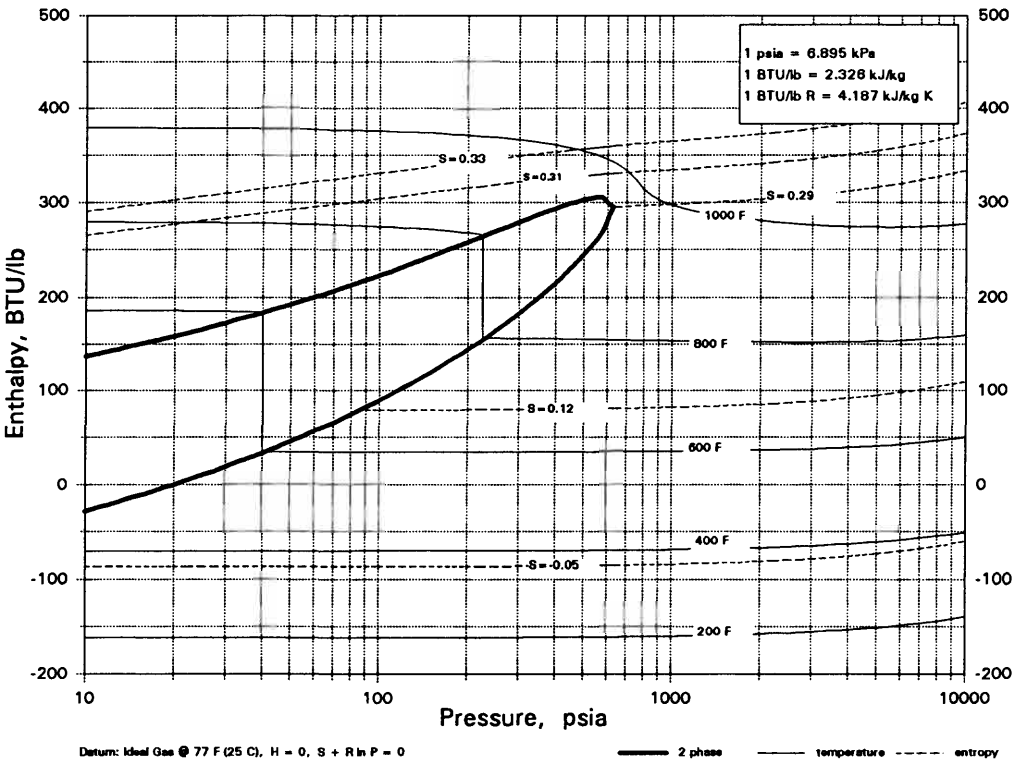
C9H7N QUINOLINE



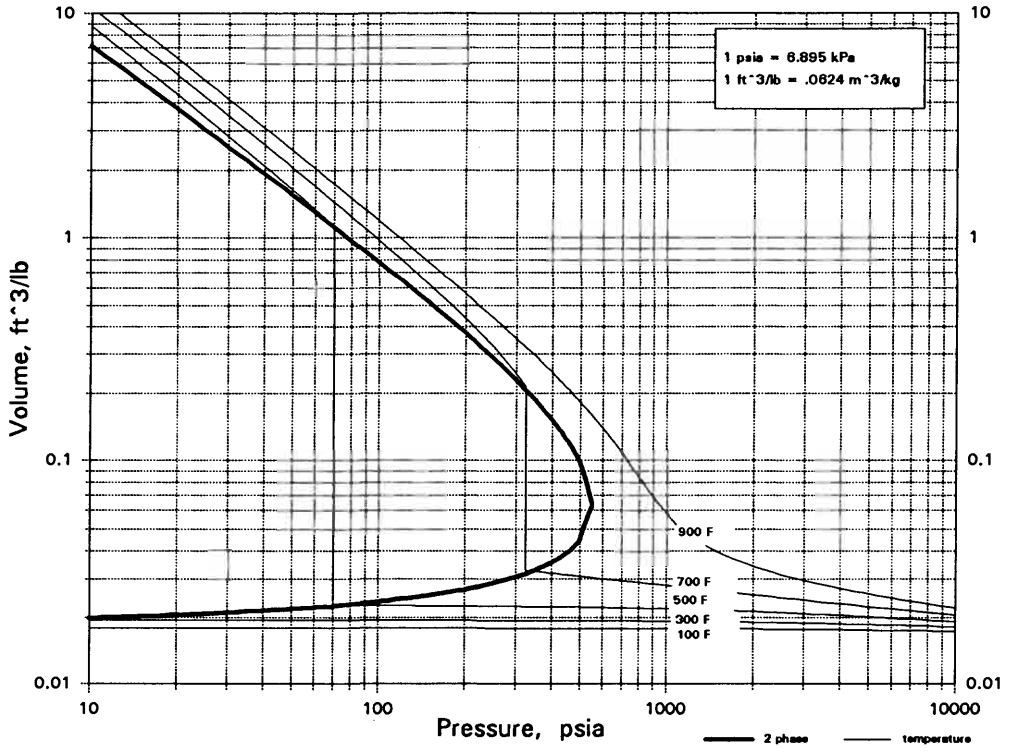


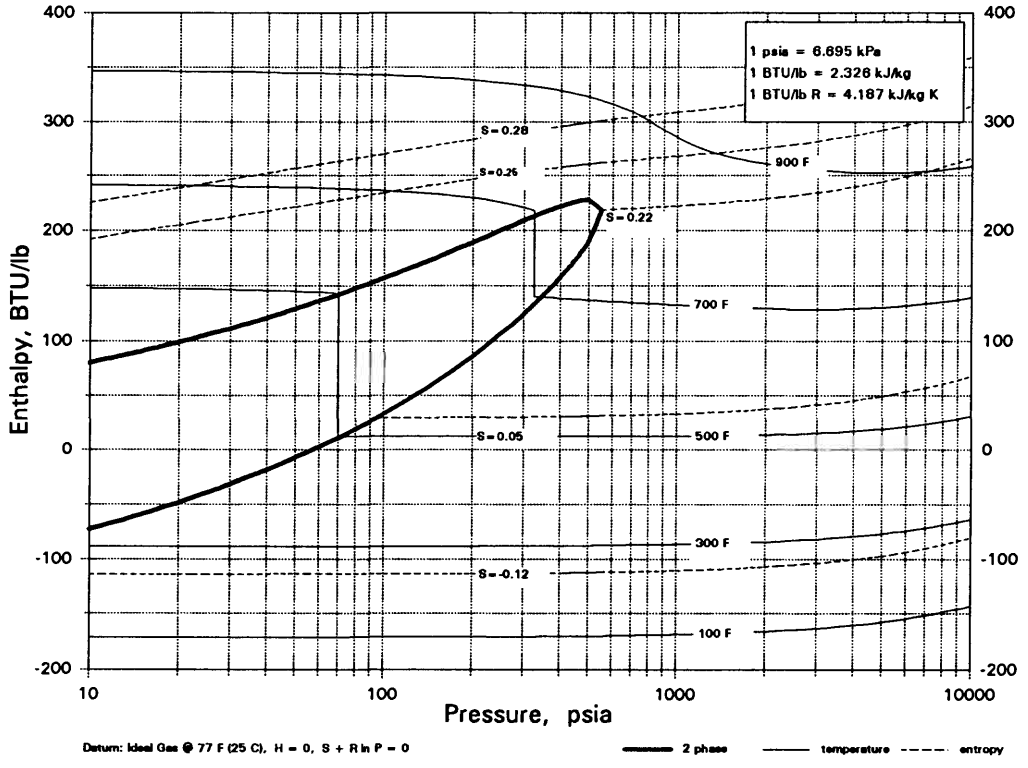
C9H7NO 8-HYDROXYQUINOLINE



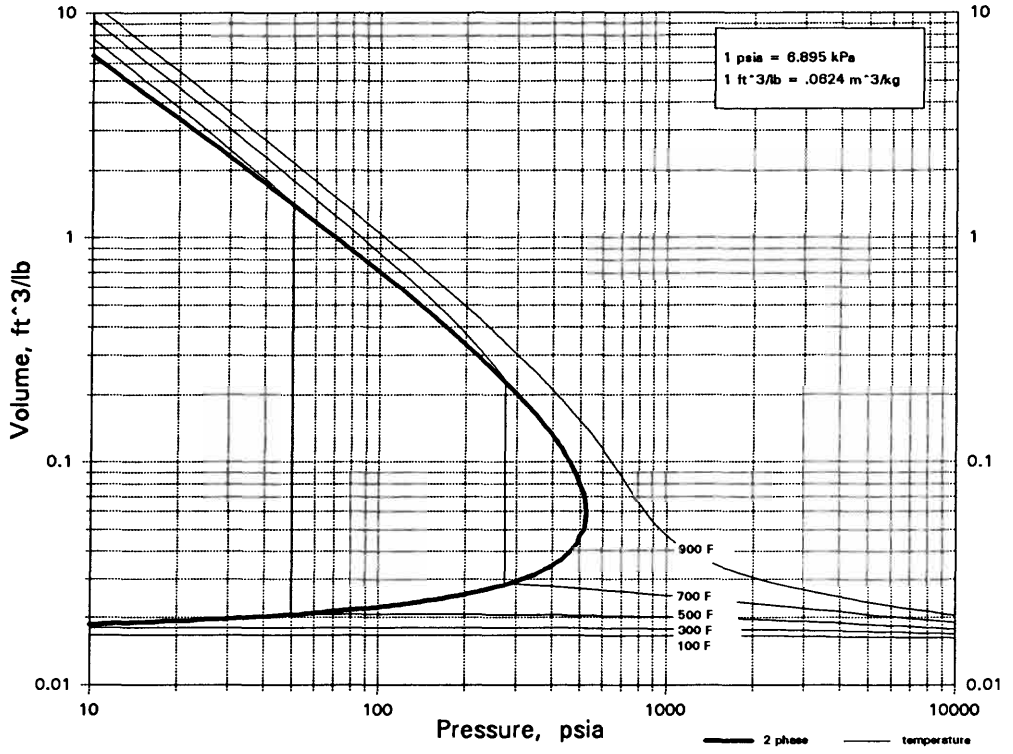


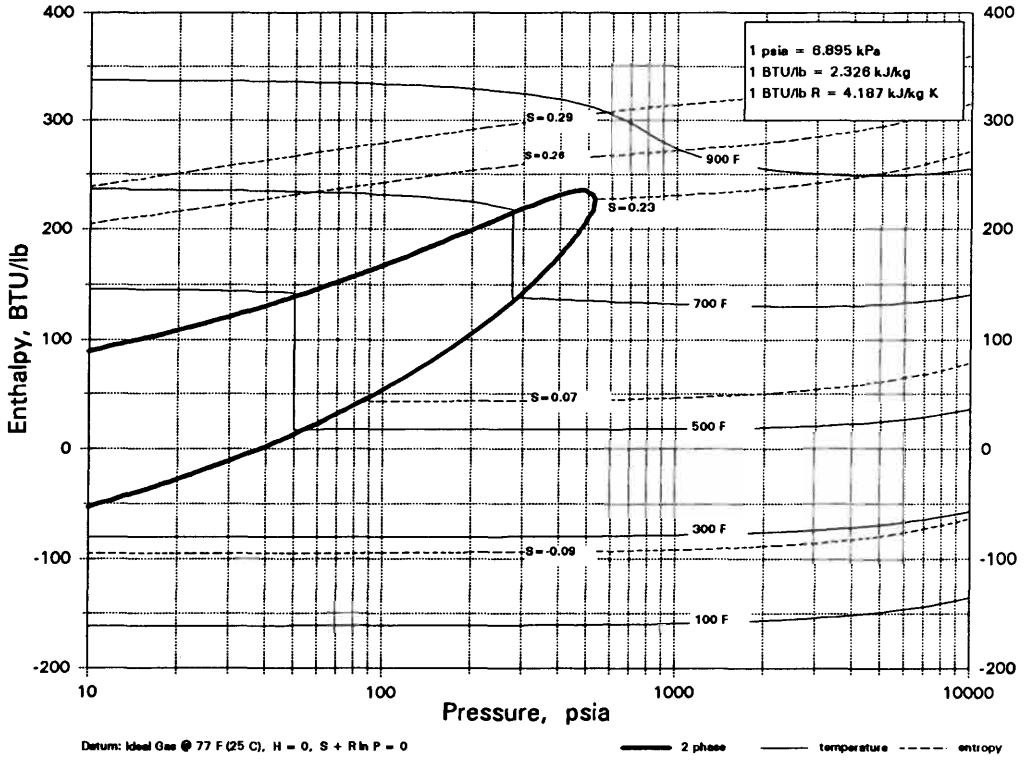
C9H8 INDENE


1 psia = 6.895 kPa
1 ft^3/lb = .0624 m^3/kg
Volume, ft^3/lb
Pressure, psia
900 F
700 F
500 F
300 F
100 F
2 phase
temperature

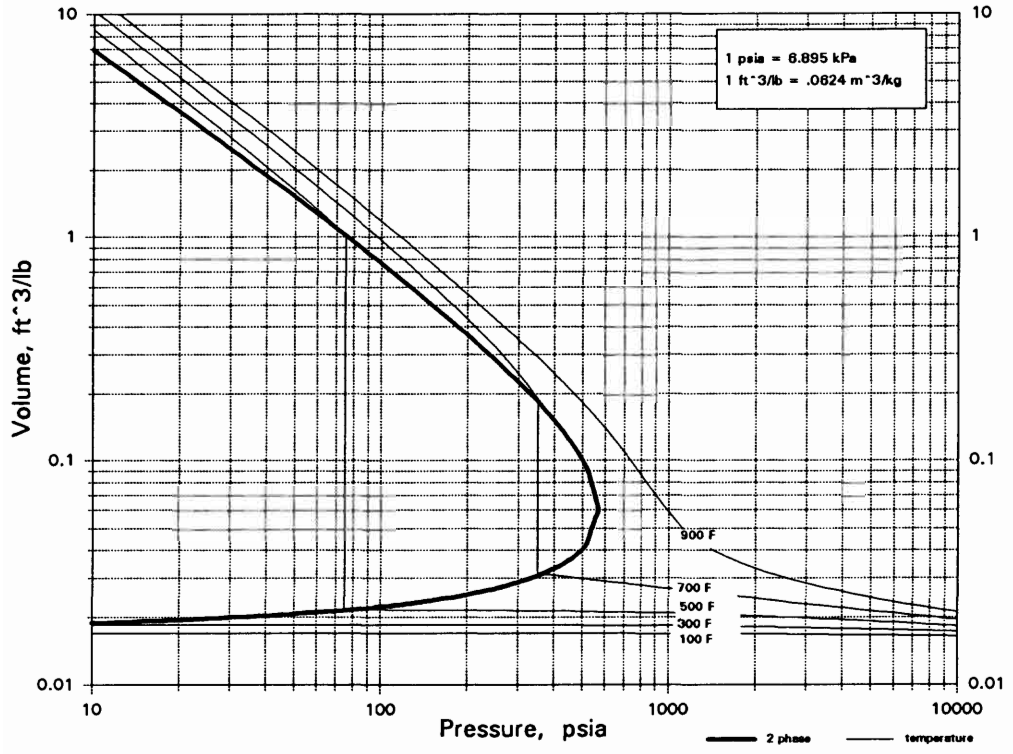

1 psia = 6.895 kPa
1 BTU/lb = 2.326 kJ/kg
1 BTU/lb R = 4.187 kJ/kg K
Enthalpy, BTU/lb
Pressure, psia
S=0.28
S=0.26
S=0.22
S=0.05
S=-0.12
900 F
700 F
500 F
300 F
100 F
Datum: Ideal Gas @ 77 F (25 C), H = 0, S + R ln P = 0
2 phase
temperature
entropy

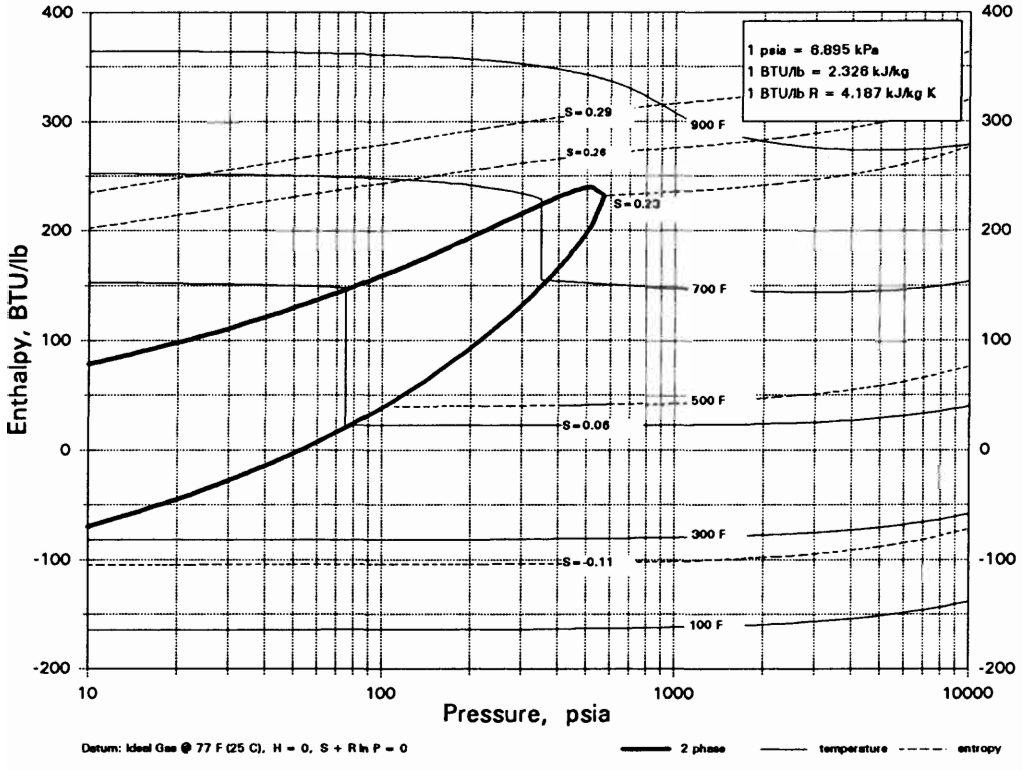
C9H8O 2-METHYLBENZOFURAN



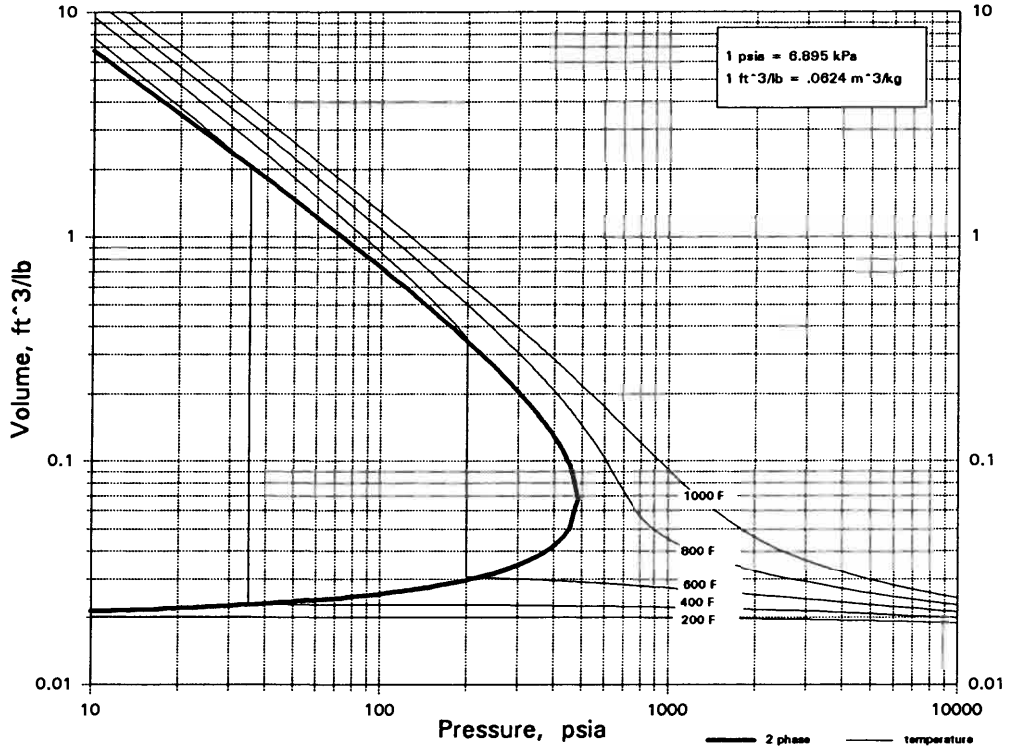


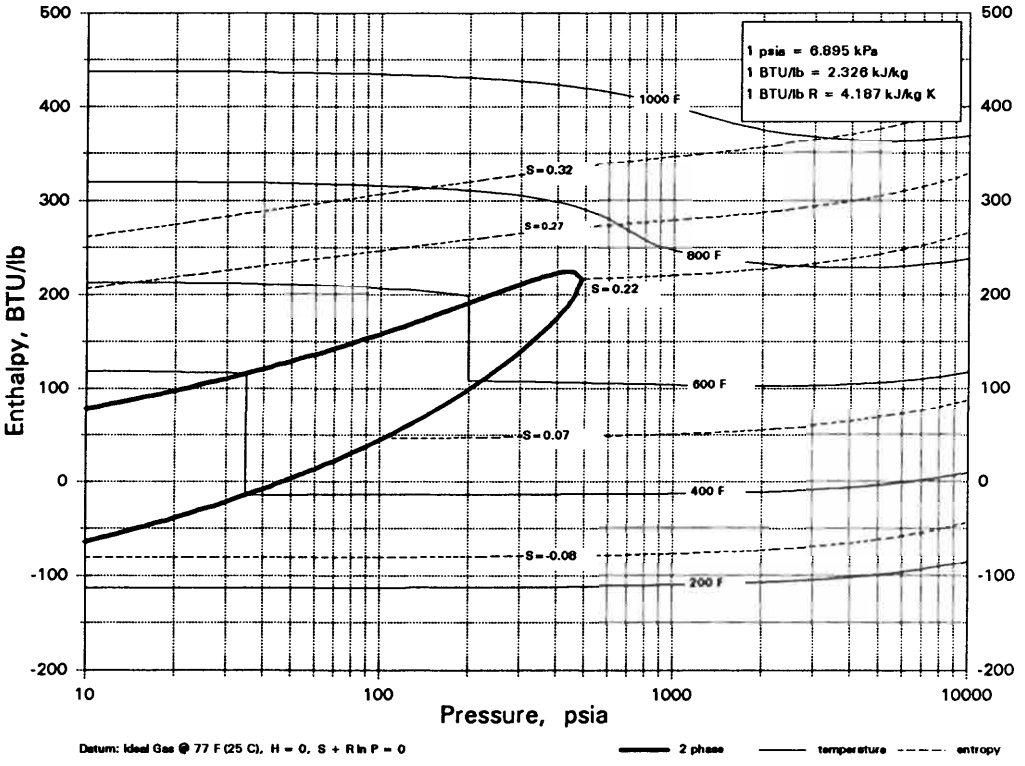
C9H10 INDANE



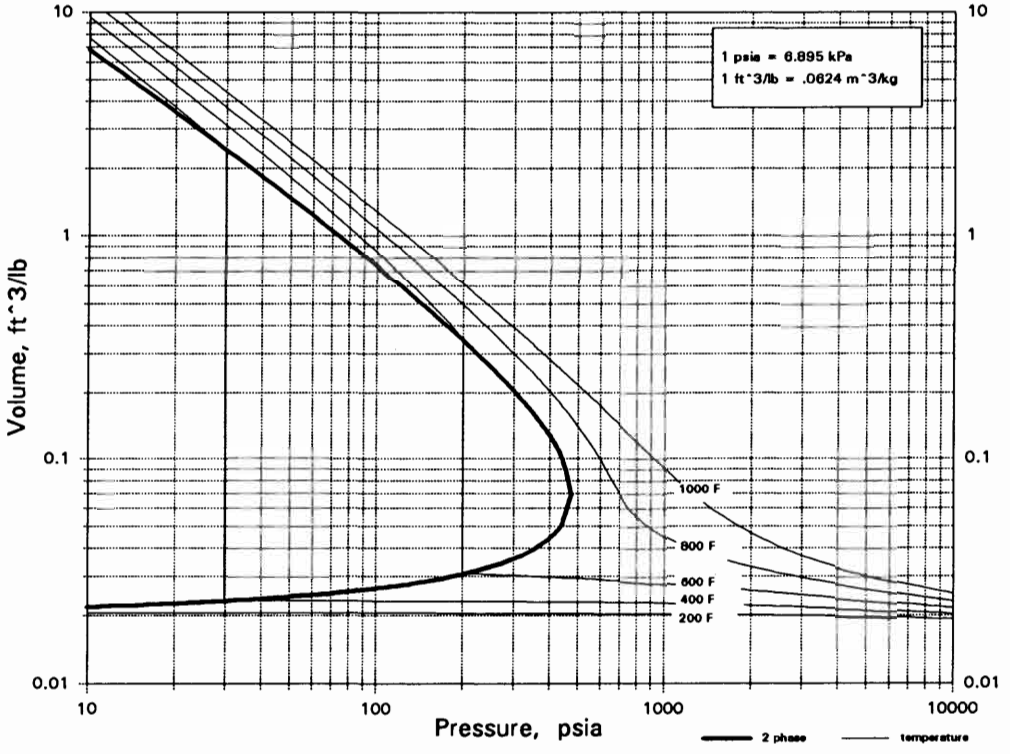


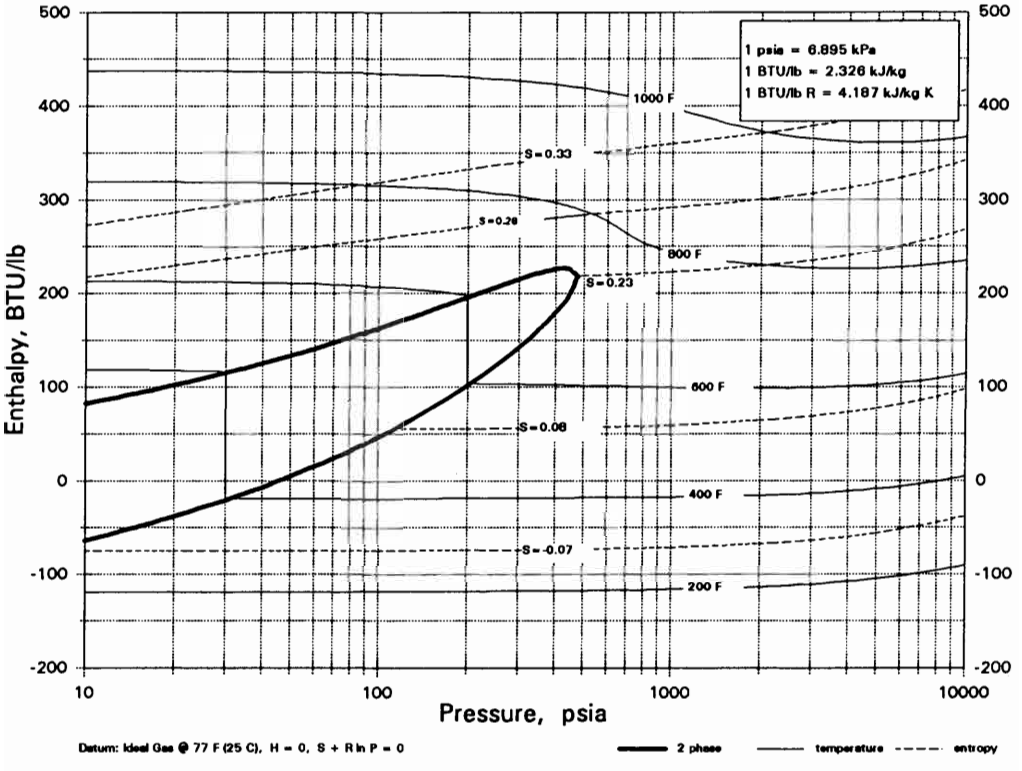
C9H1O alpha-METHYLSTYRENE



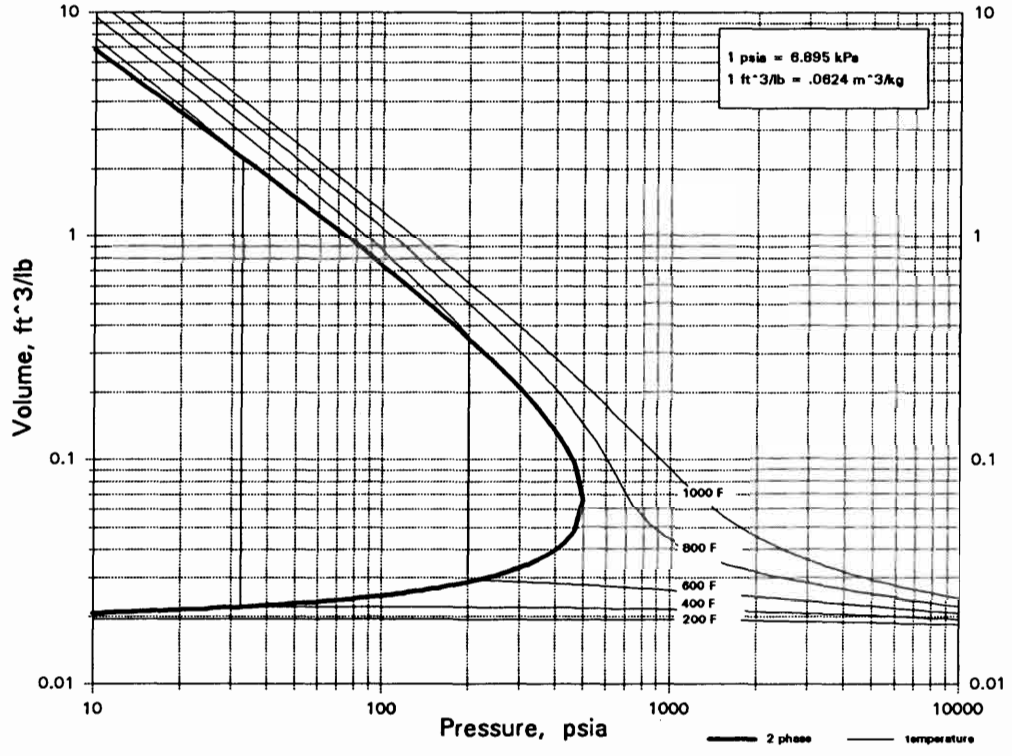


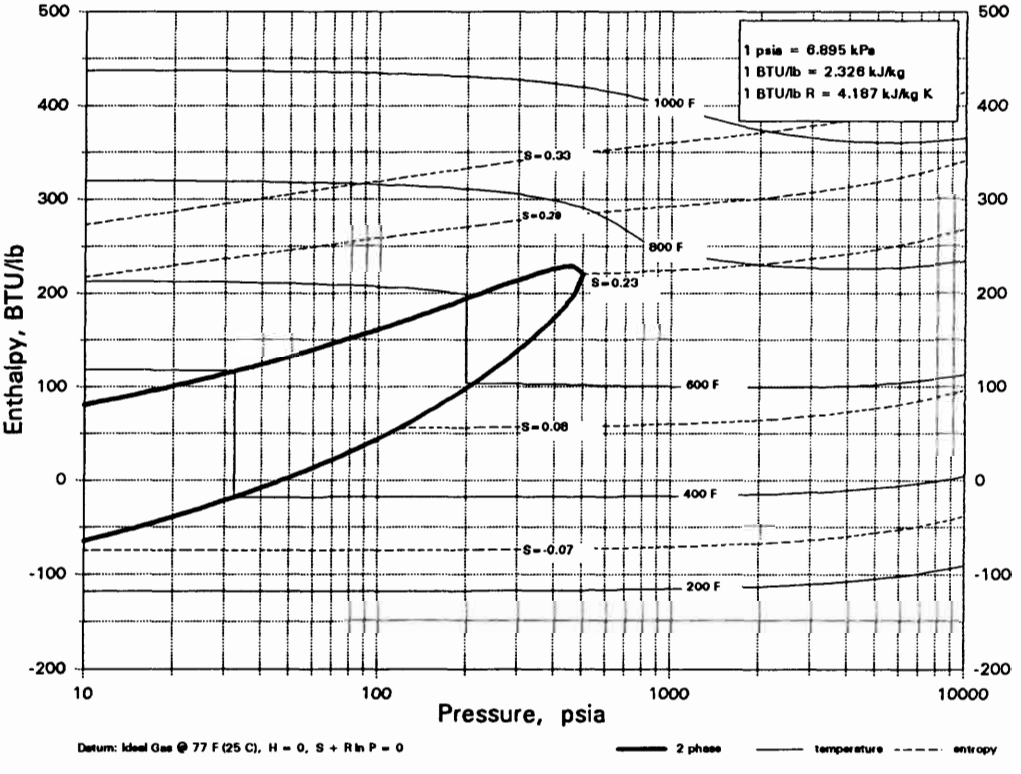
C9H10 m-METHYLSTYRENE



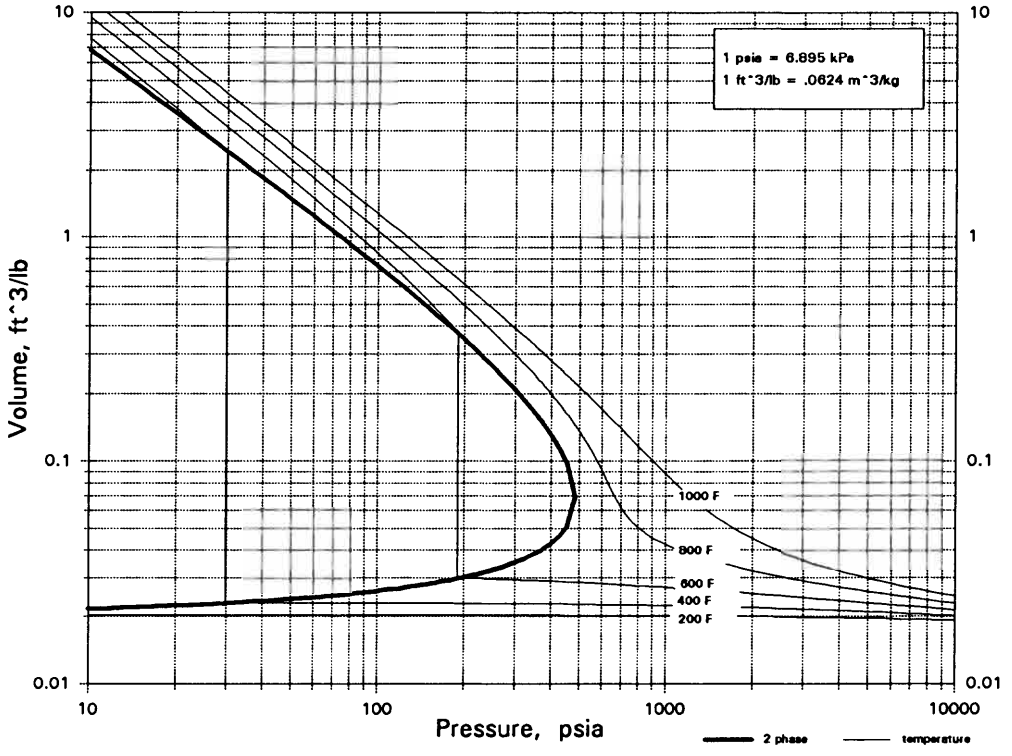


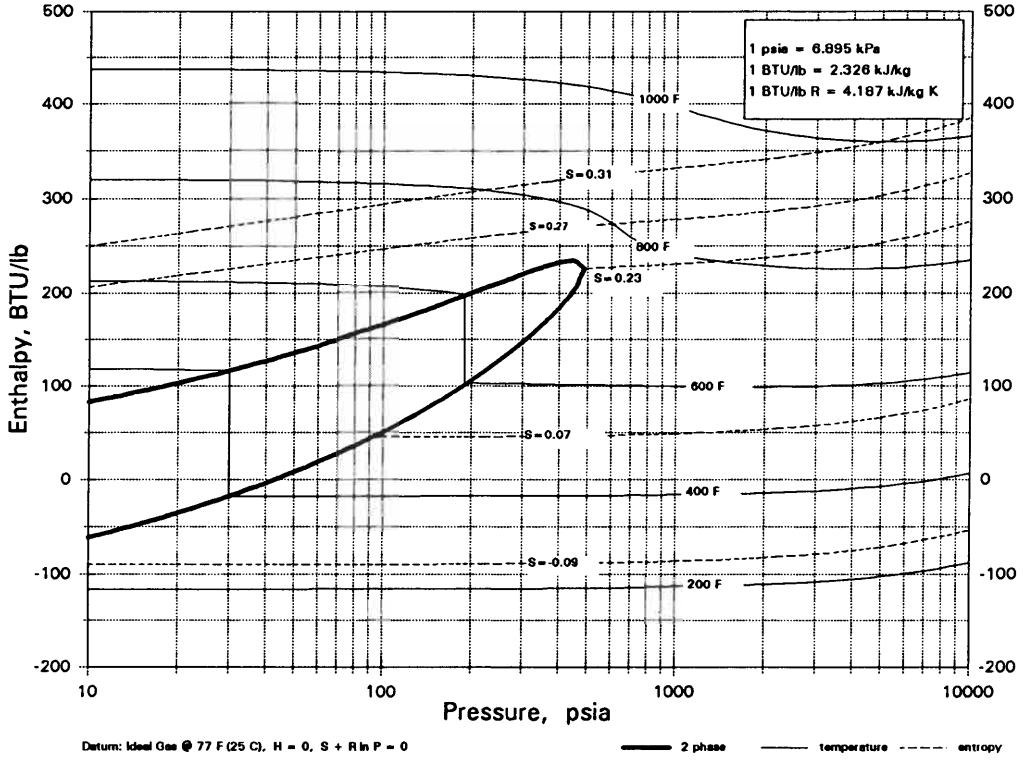
C9H10 o-METHYLSTYRENE



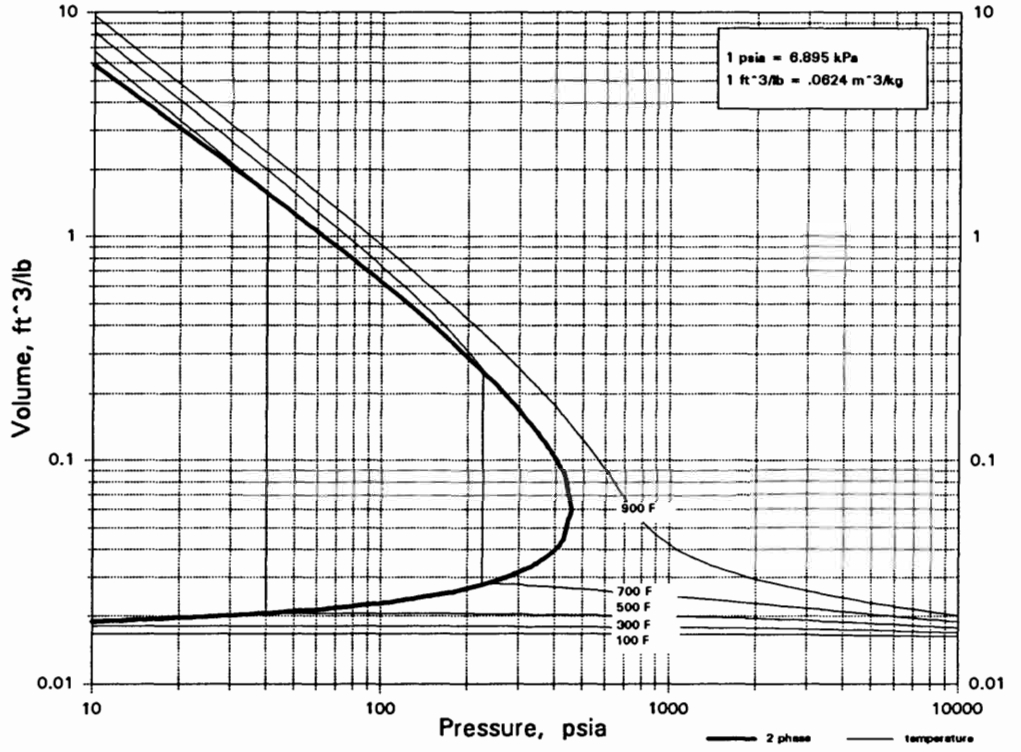


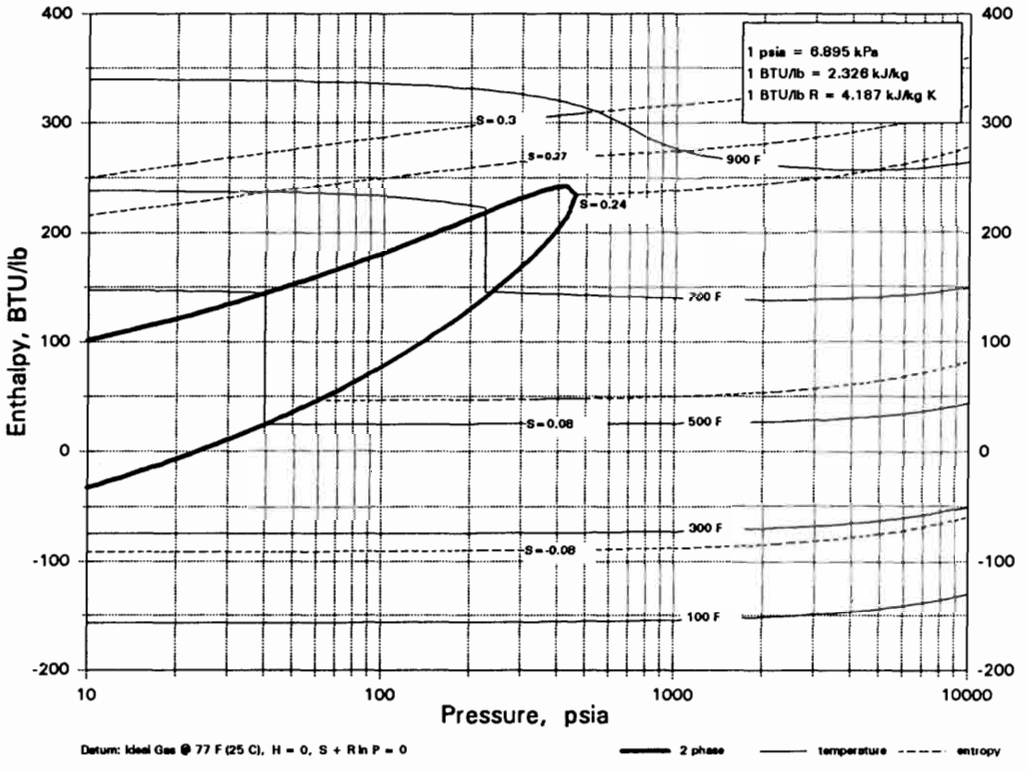
C9H10 p-METHYLSTYRENE



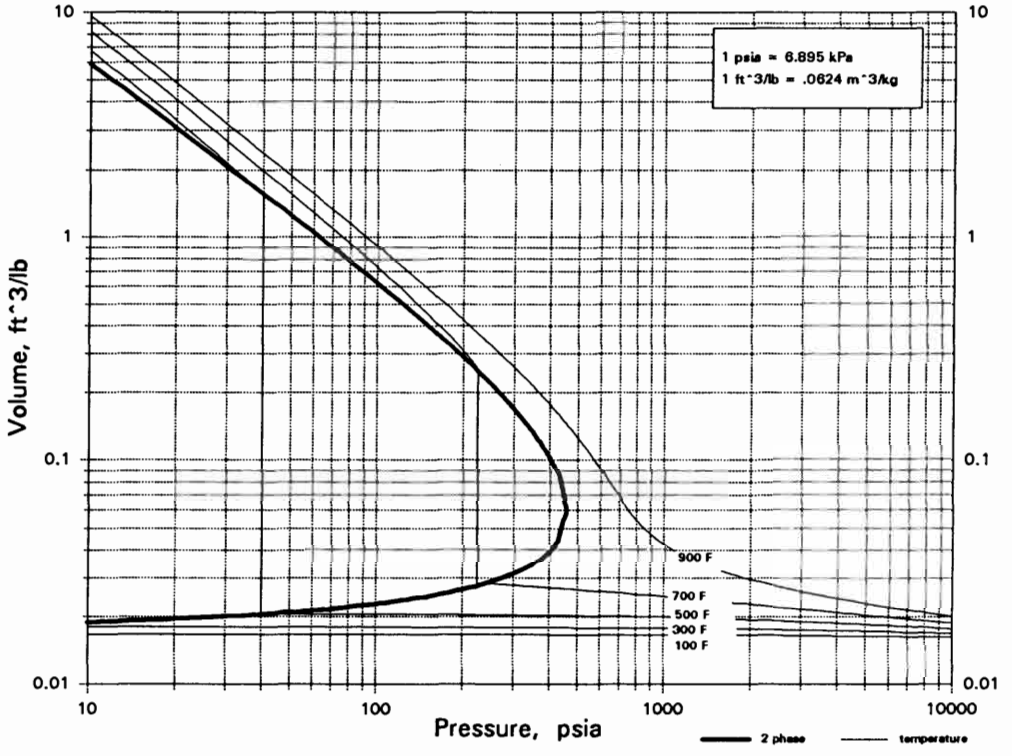


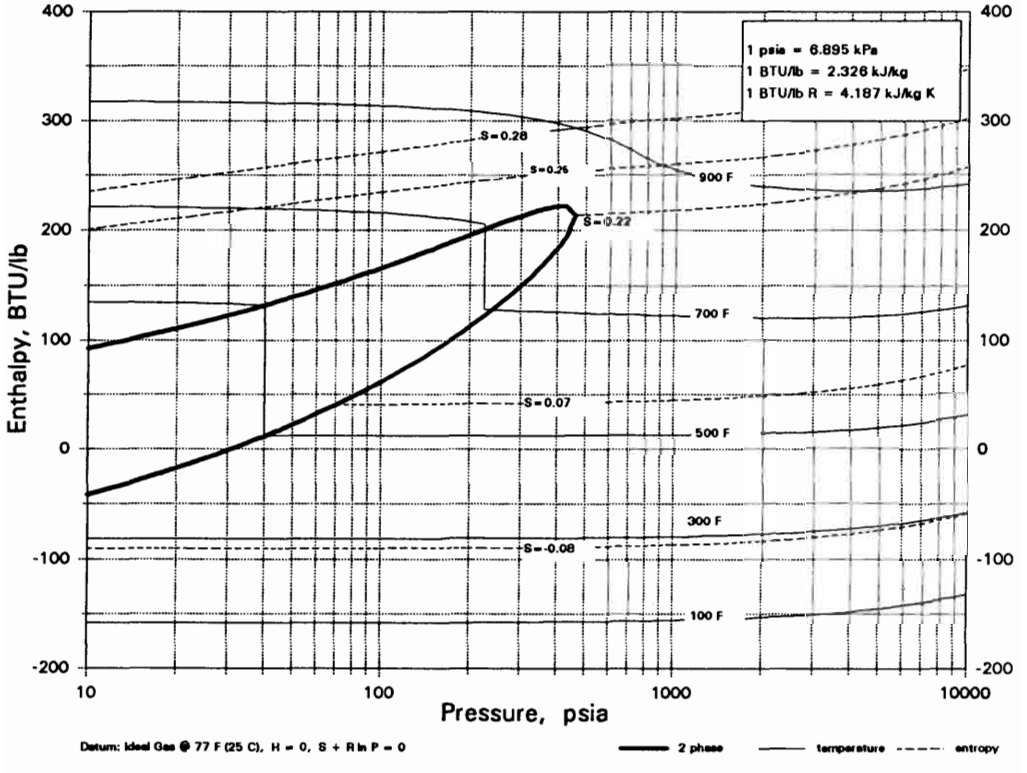
C9H10O2 BENZYL ACETATE



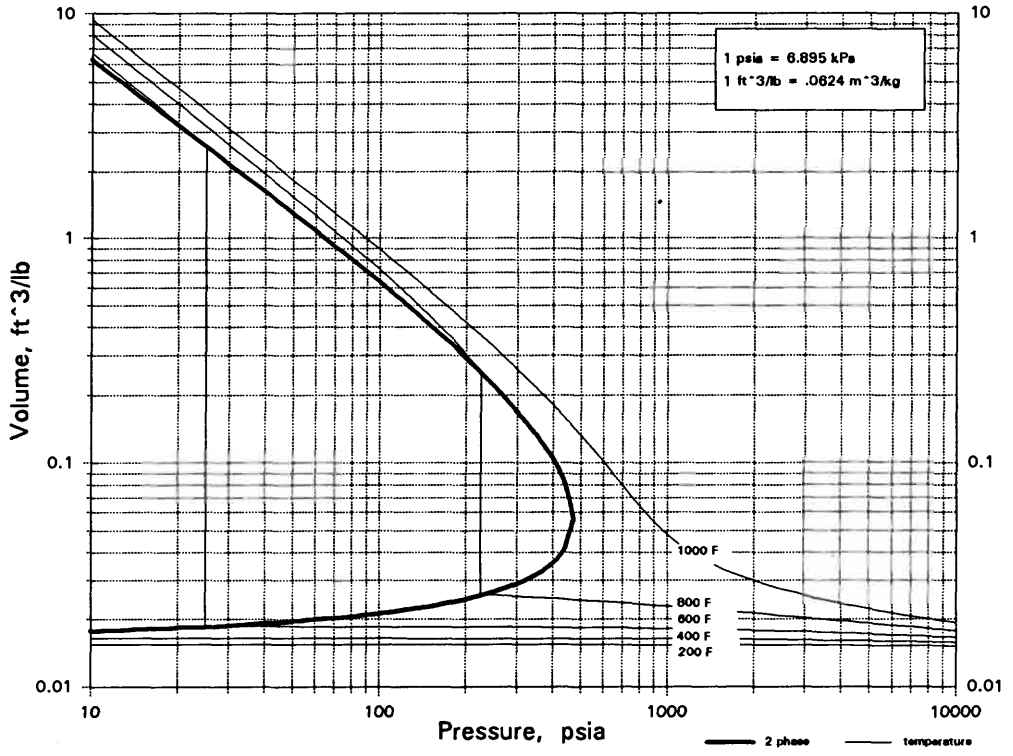


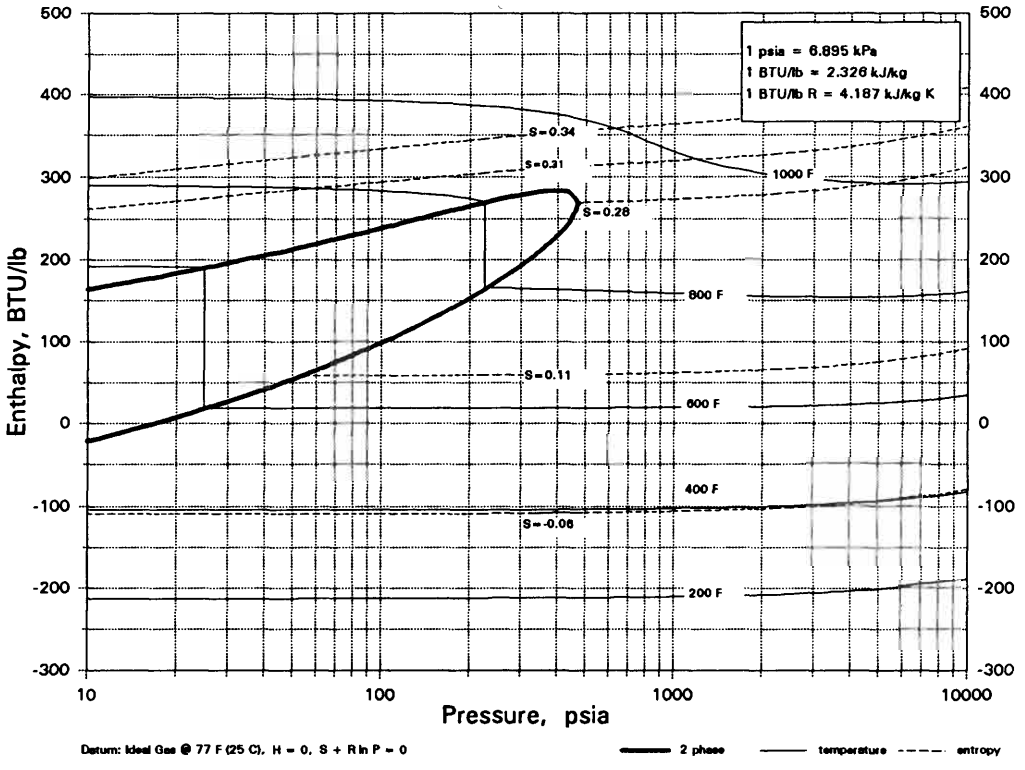
C9H10O2 ETHYL BENZOATE



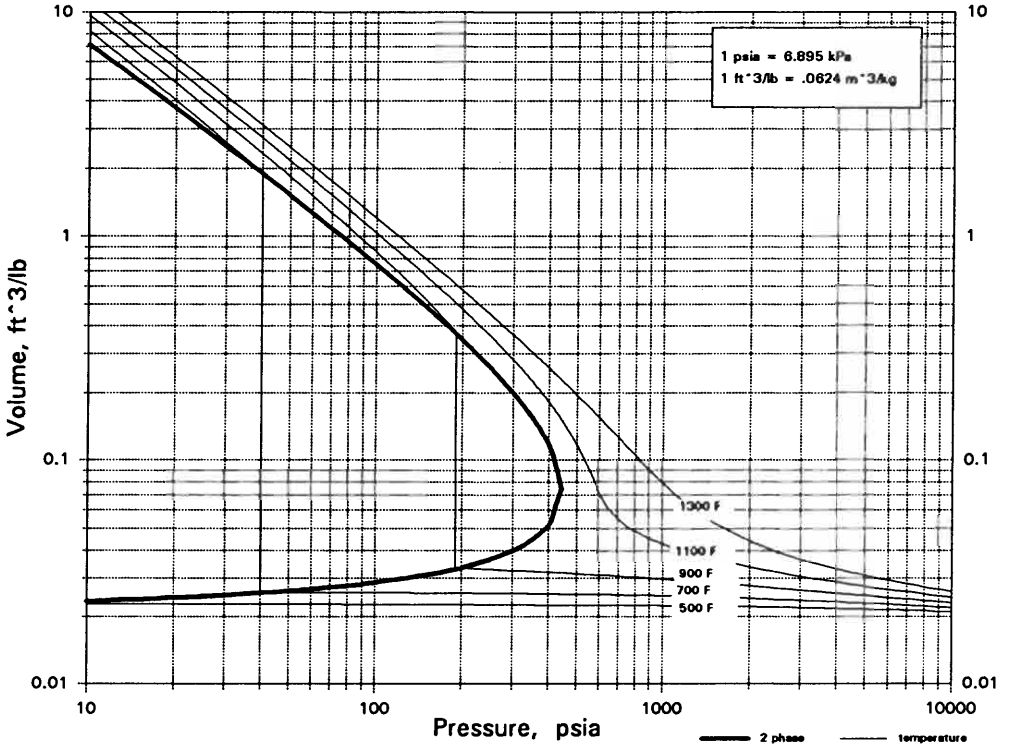


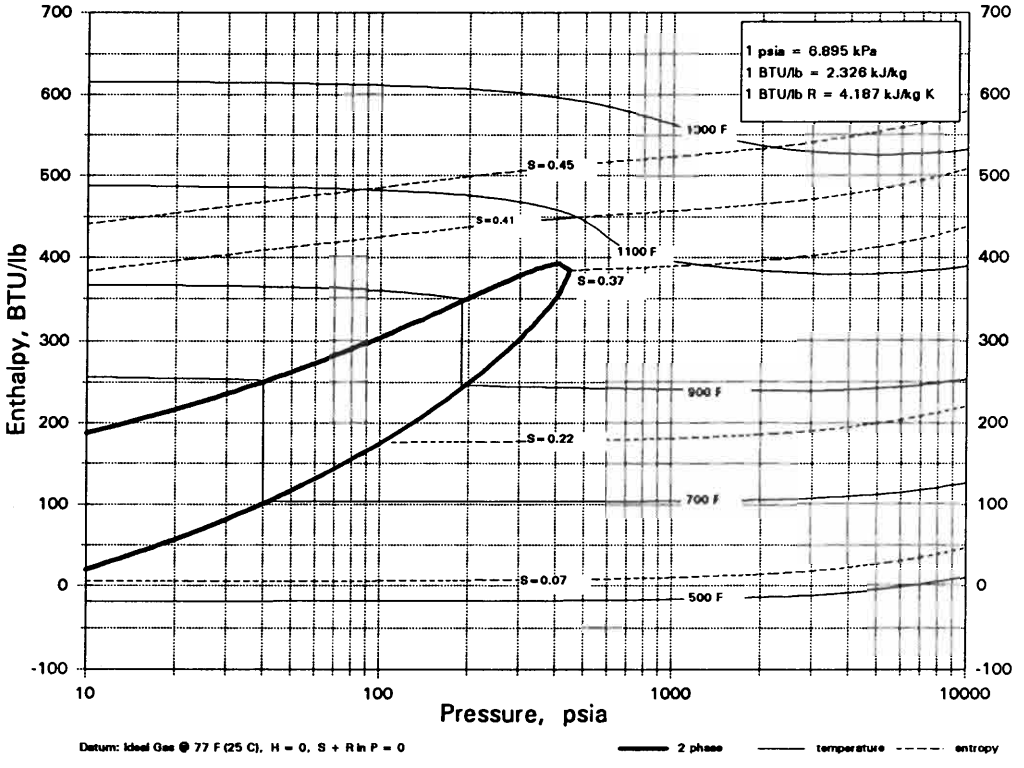
C9H10O3 ETHYL VANILLIN



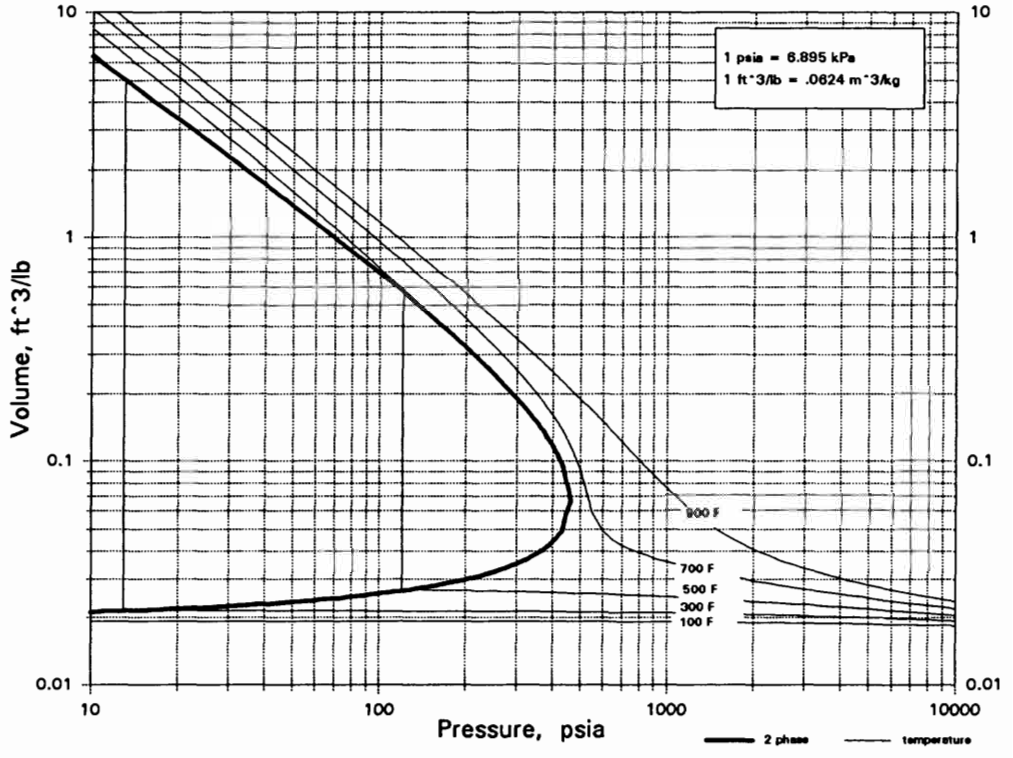


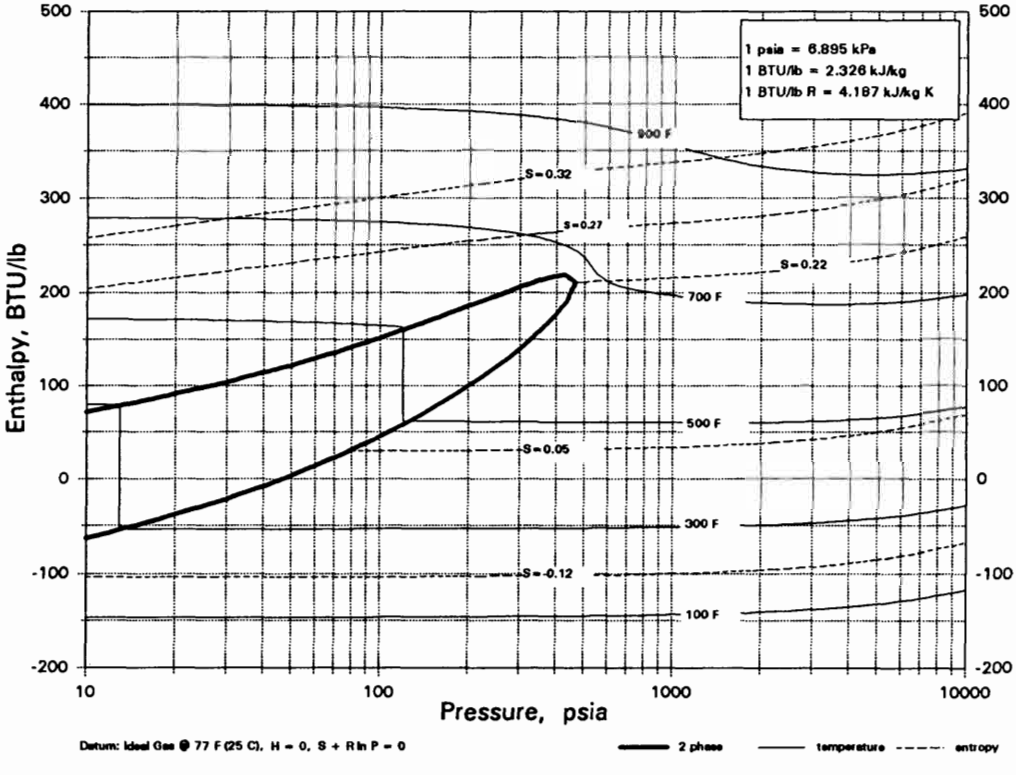
C9H11NO p-DIMETHYLAMINOBENZALDEHYDE



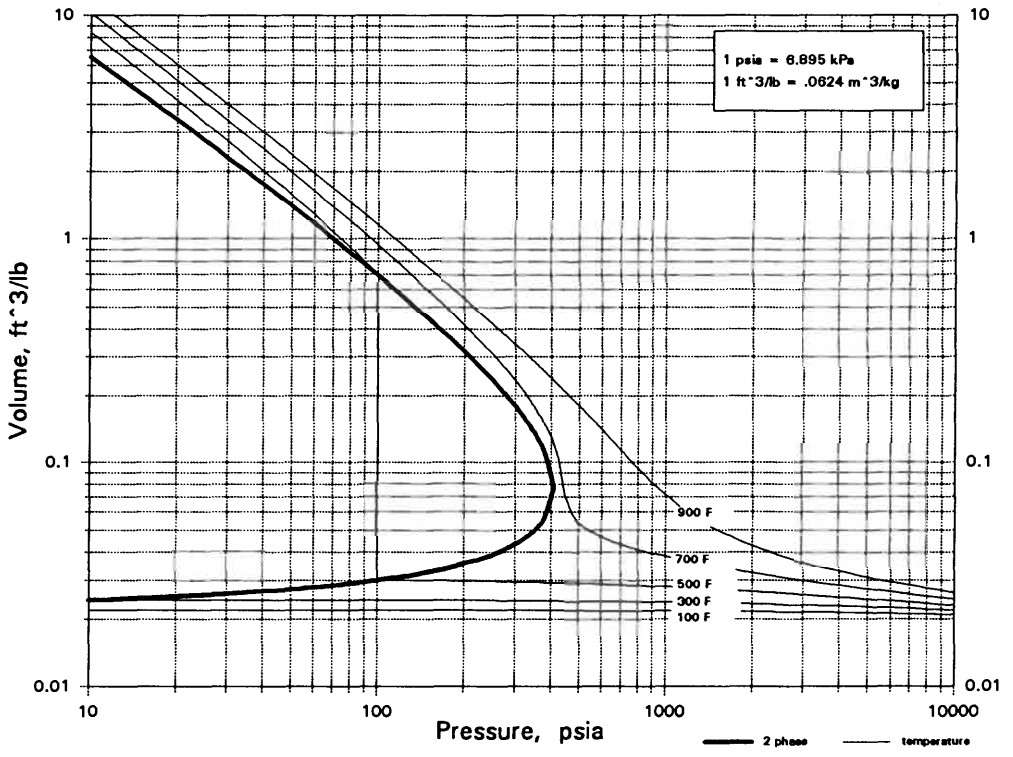


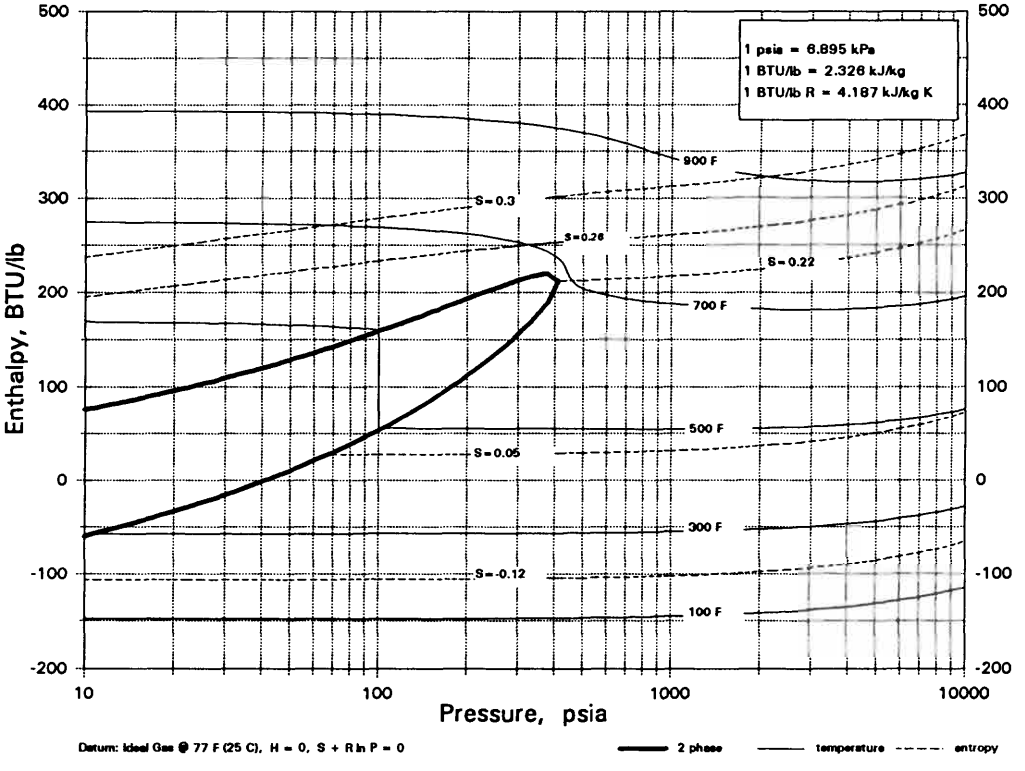
C9H12 CUMENE



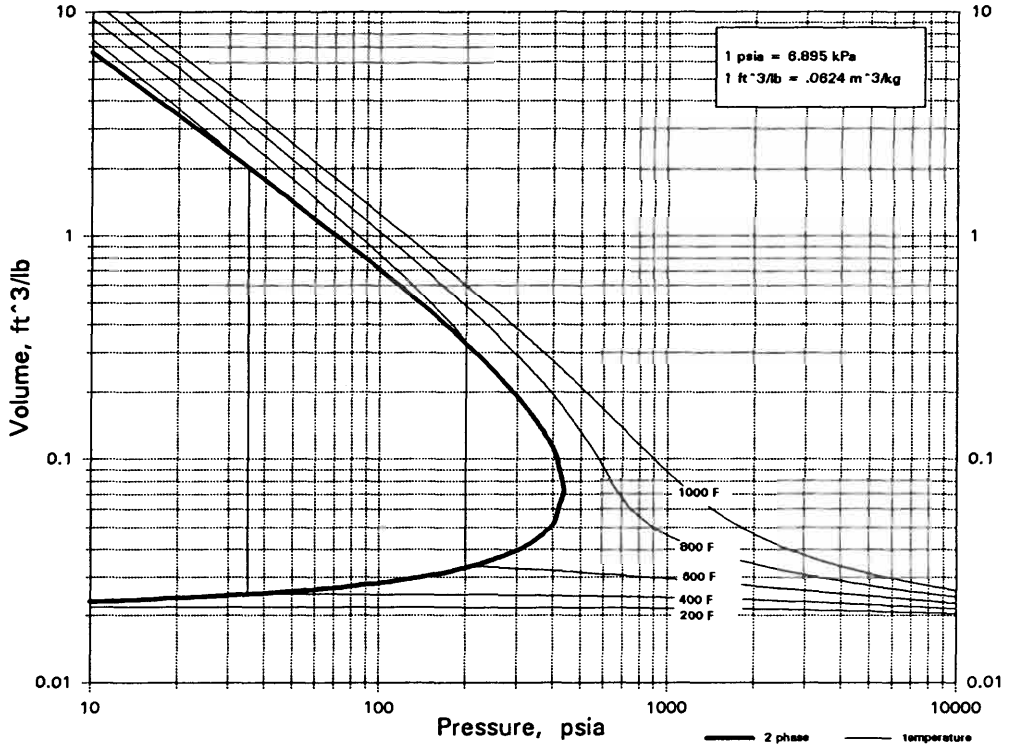


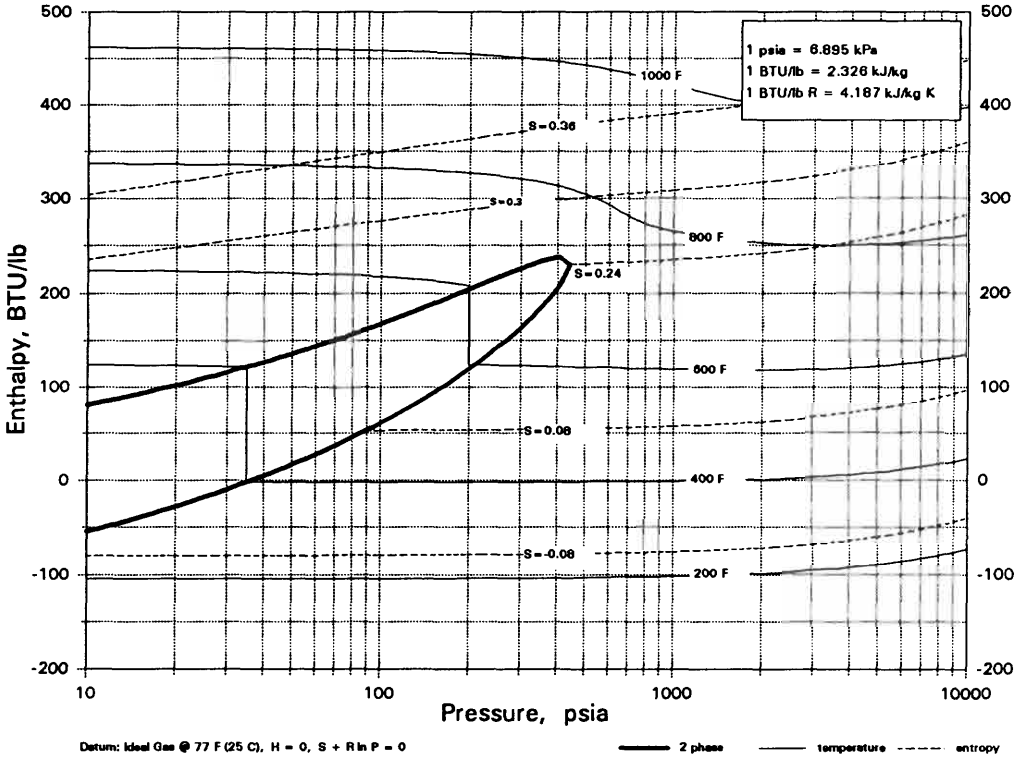
C9H12 m-ETHYLTOLUENE



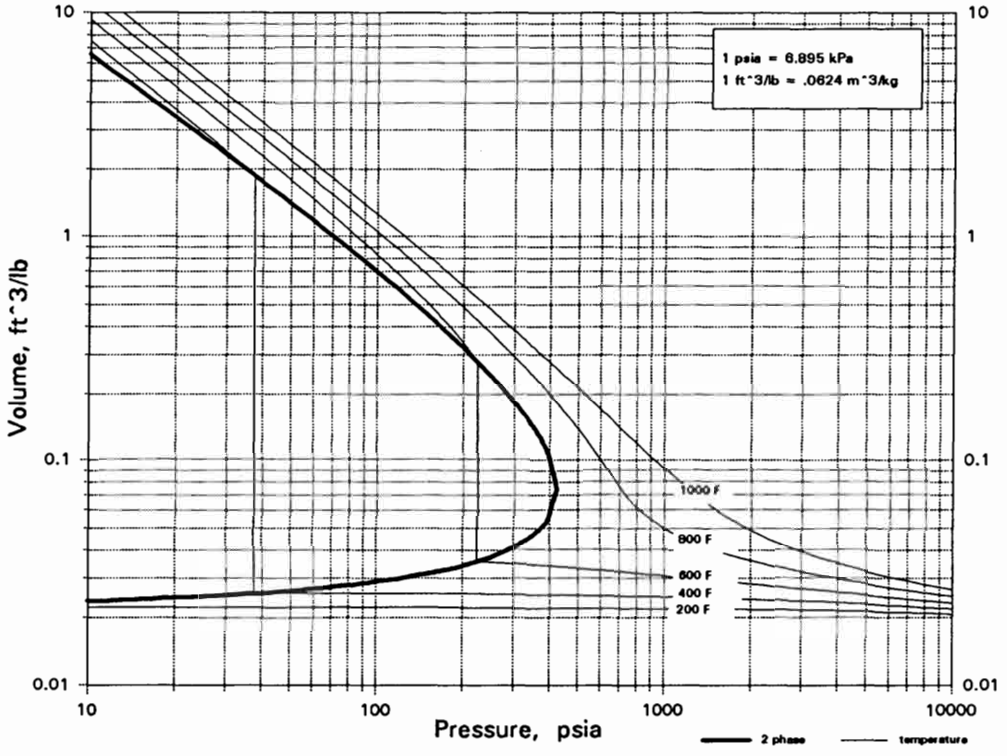


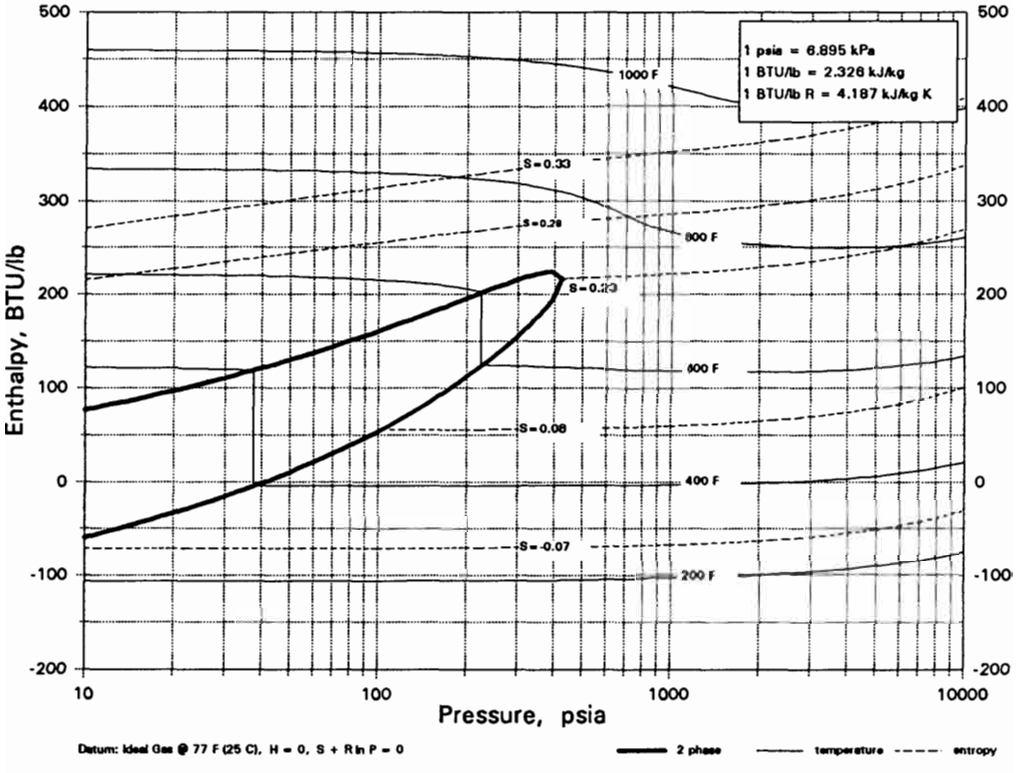
C9H12 o-ETHYLTOLUENE



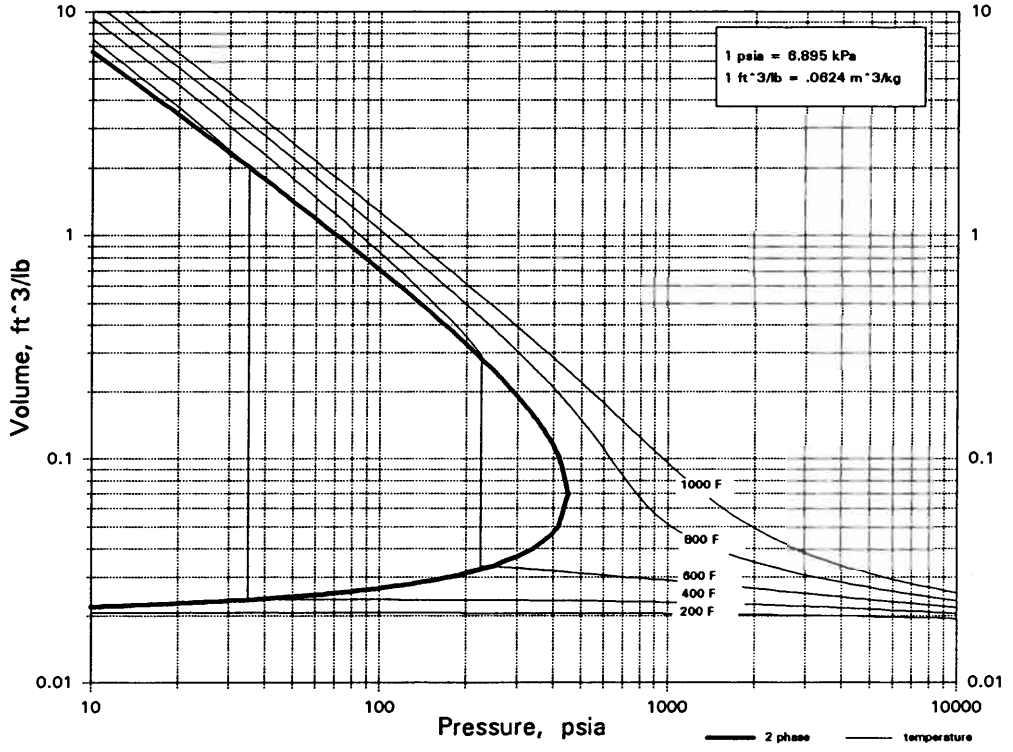


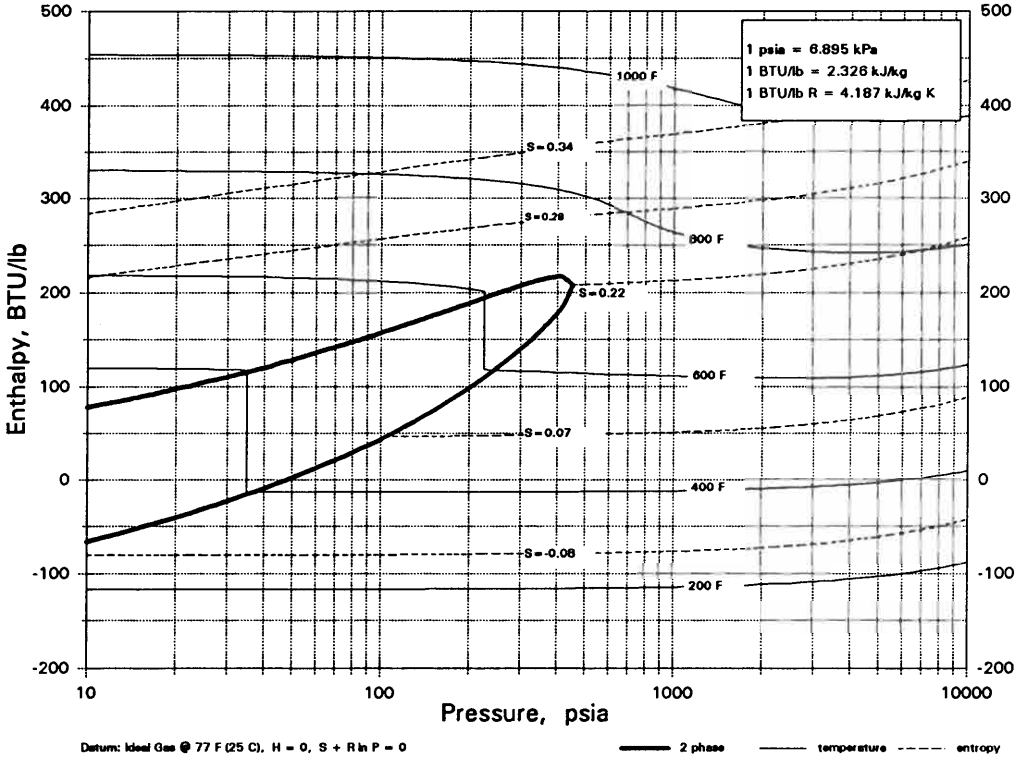
C9H12 p-ETHYLTOLUENE



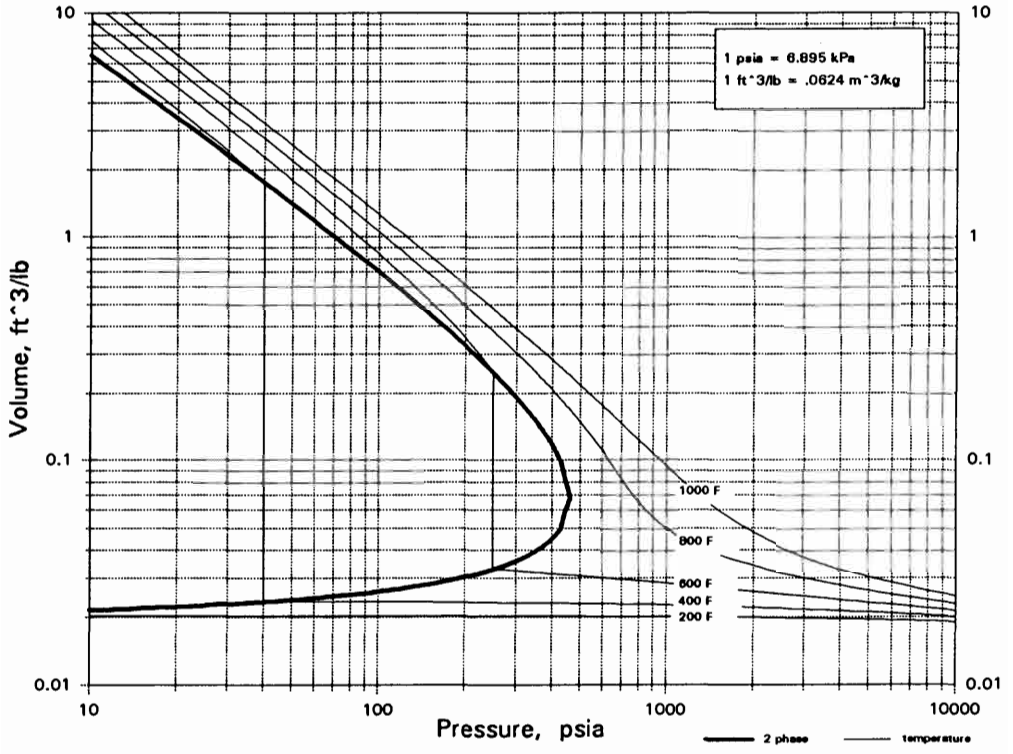


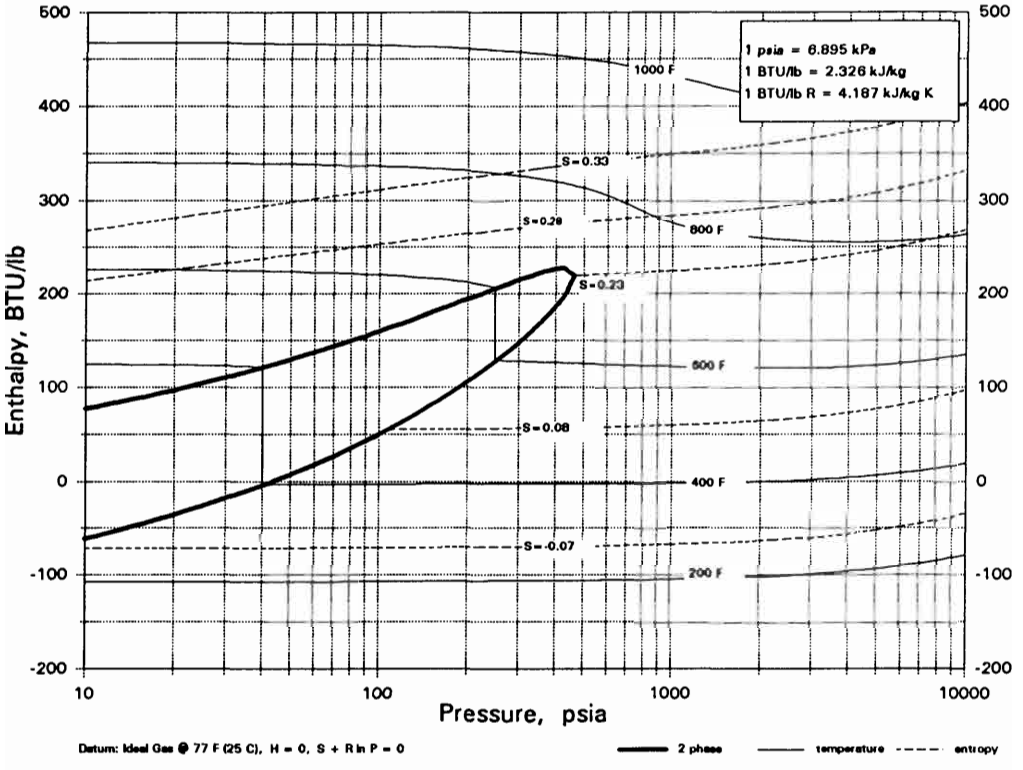
C9H12 MESITYLENE



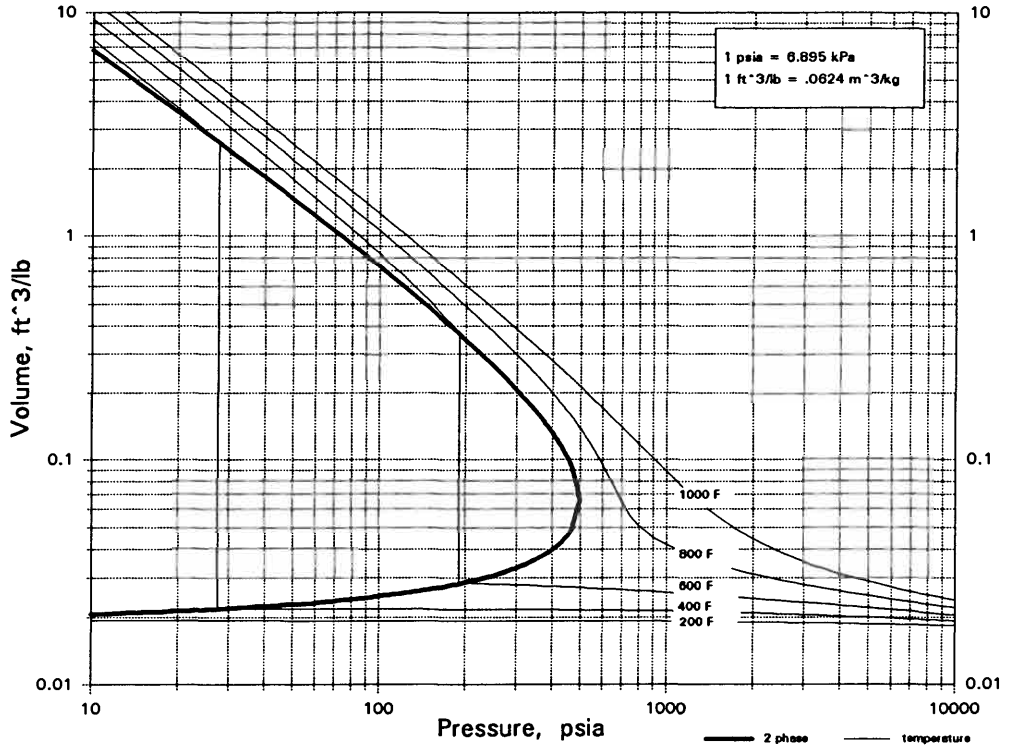


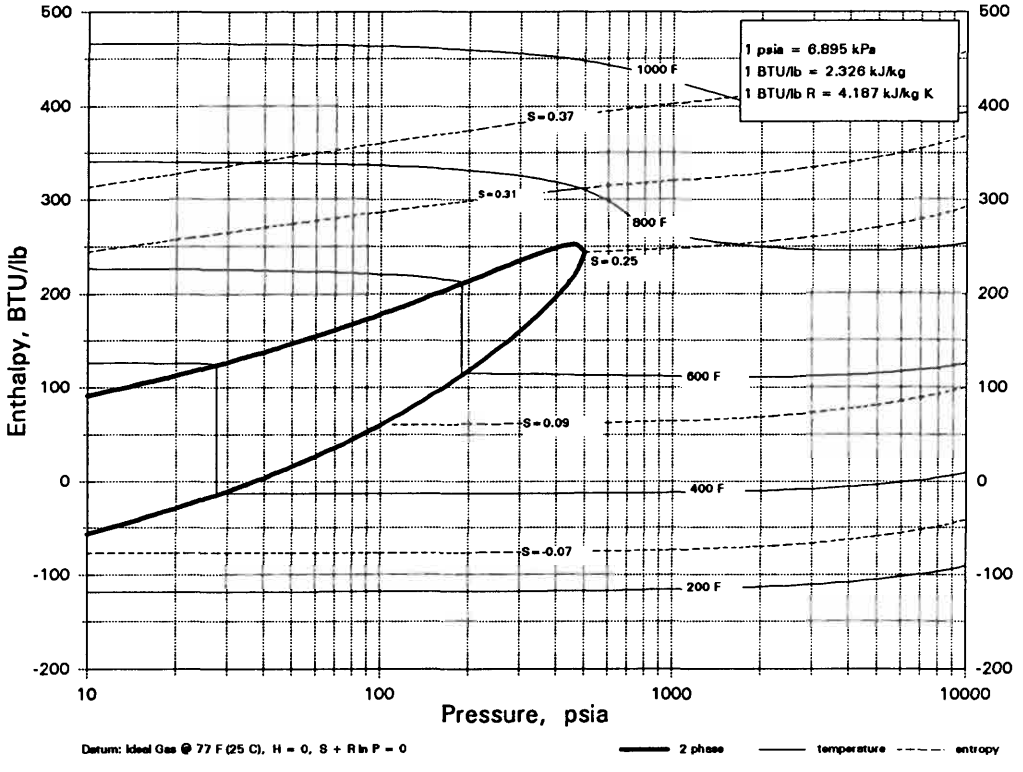
C9H12 n-PROPYLBENZENE



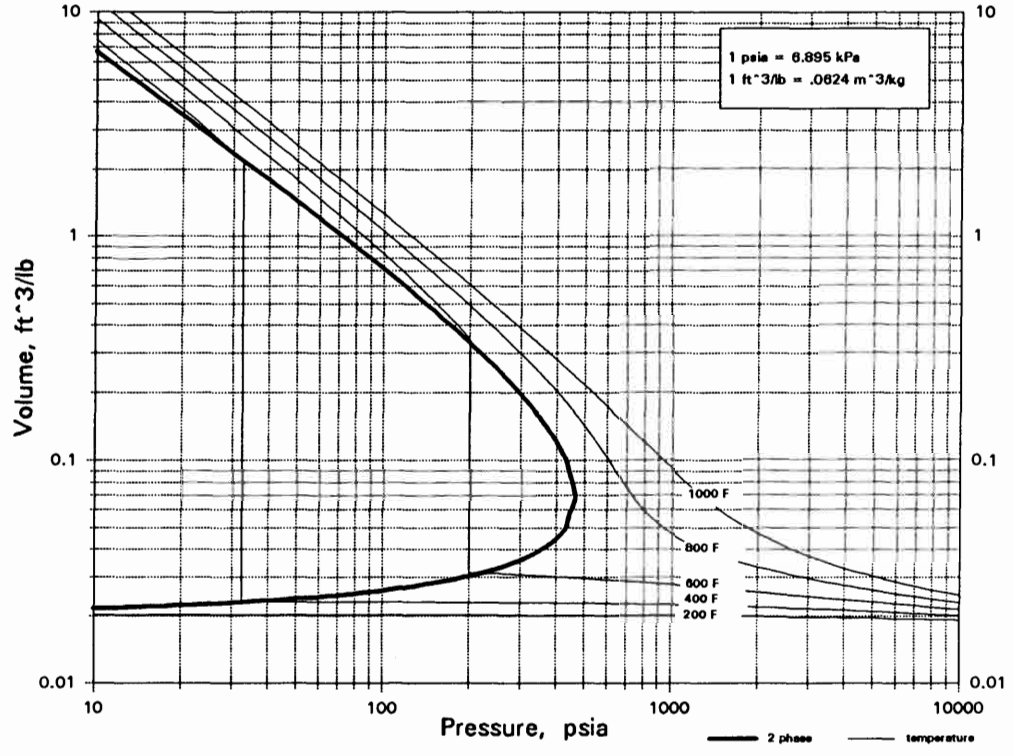


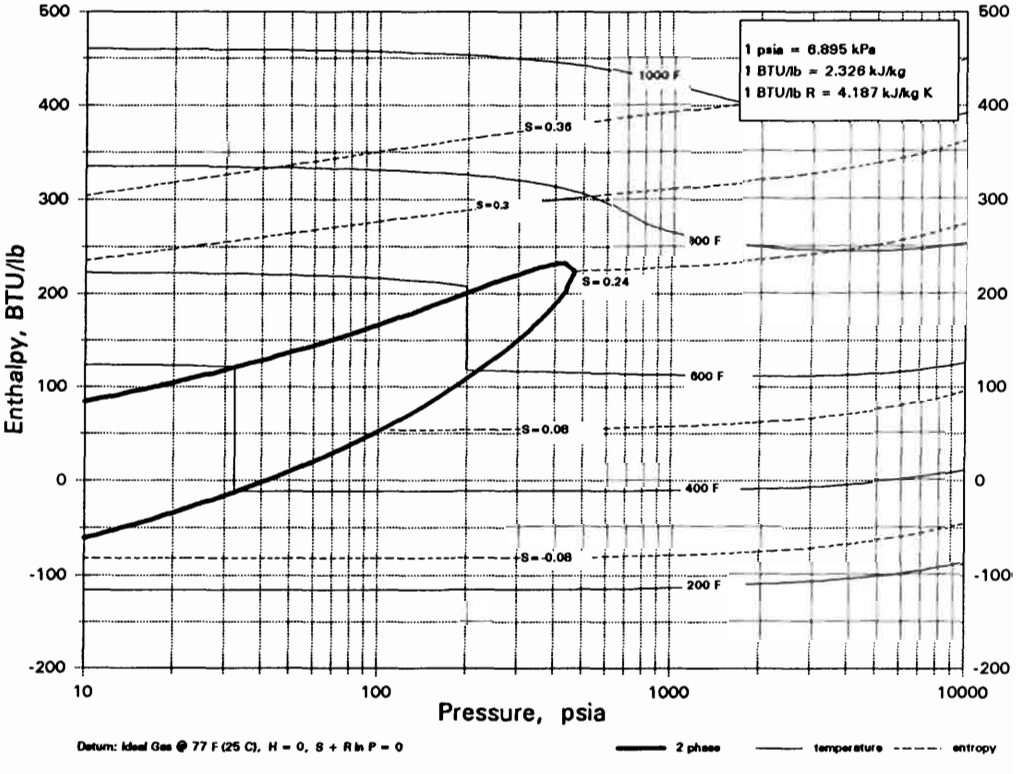
C9H12	1-2-3-TRIMETHYLBENZENE



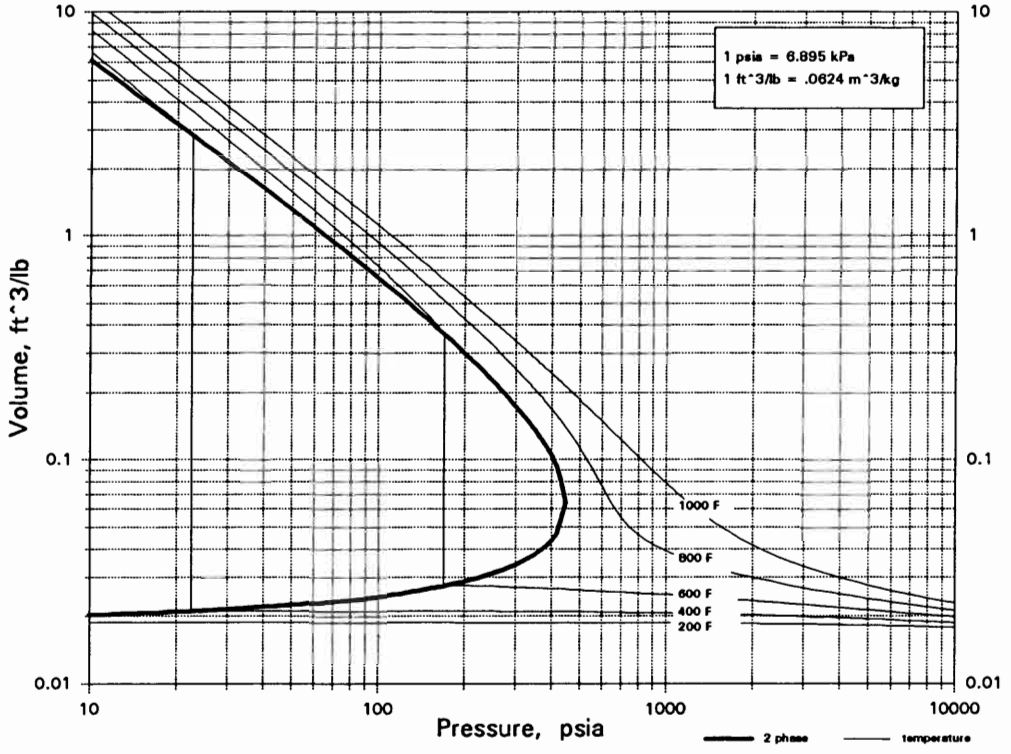


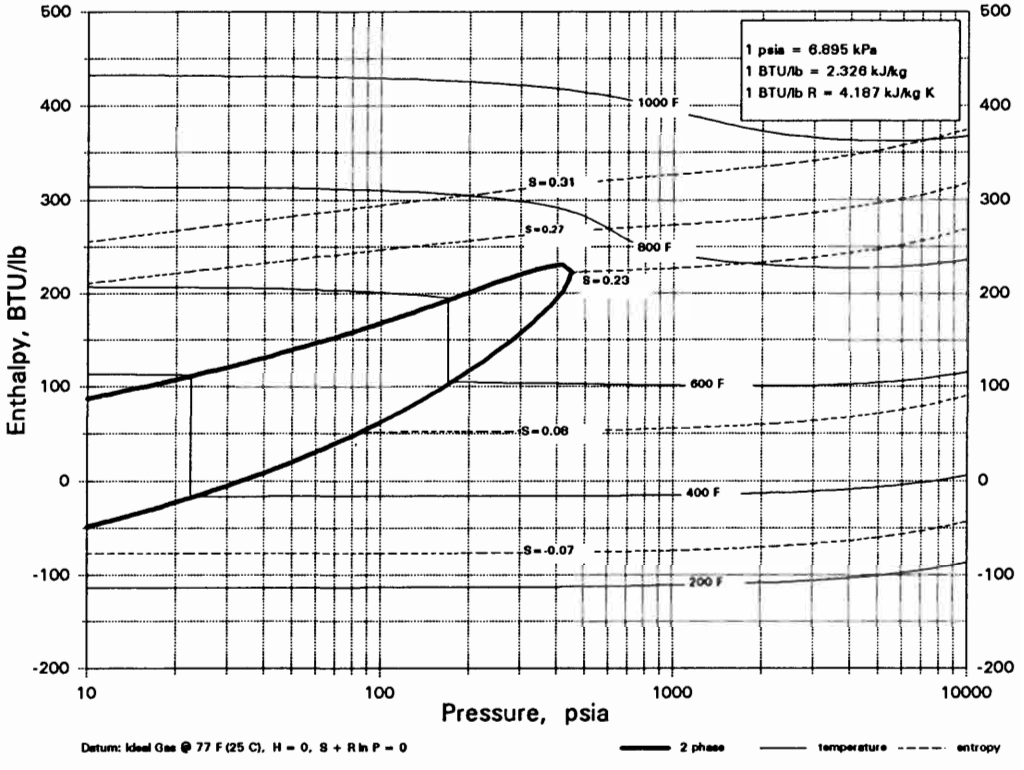
C9H12 1-2-4-TRIMETHYLBENZENE



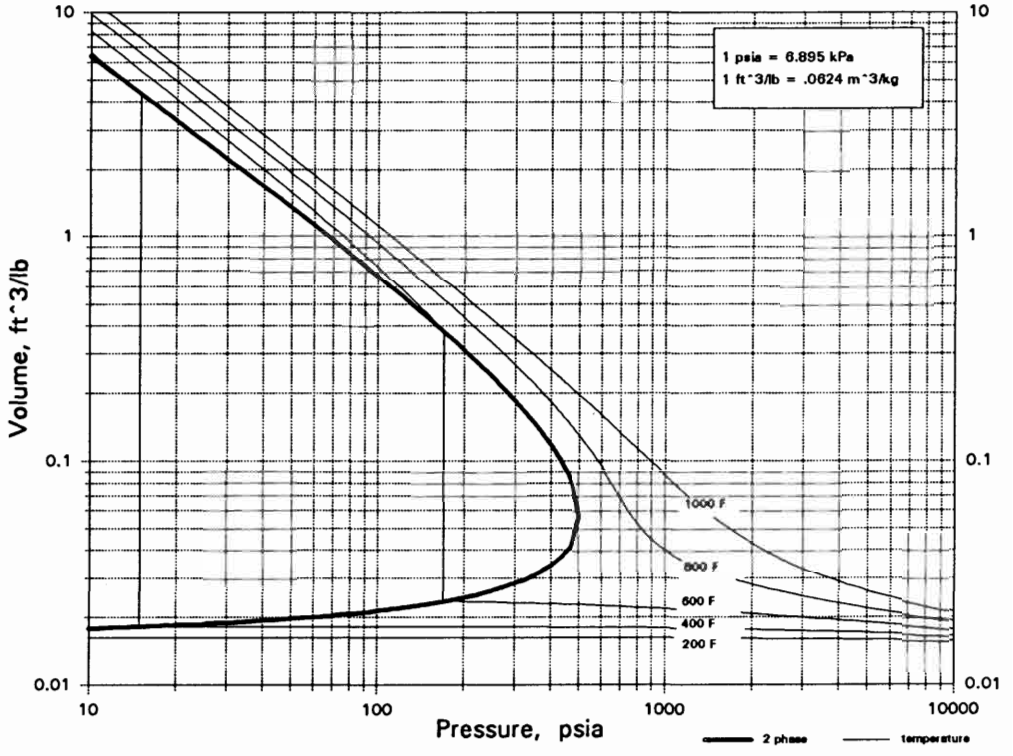


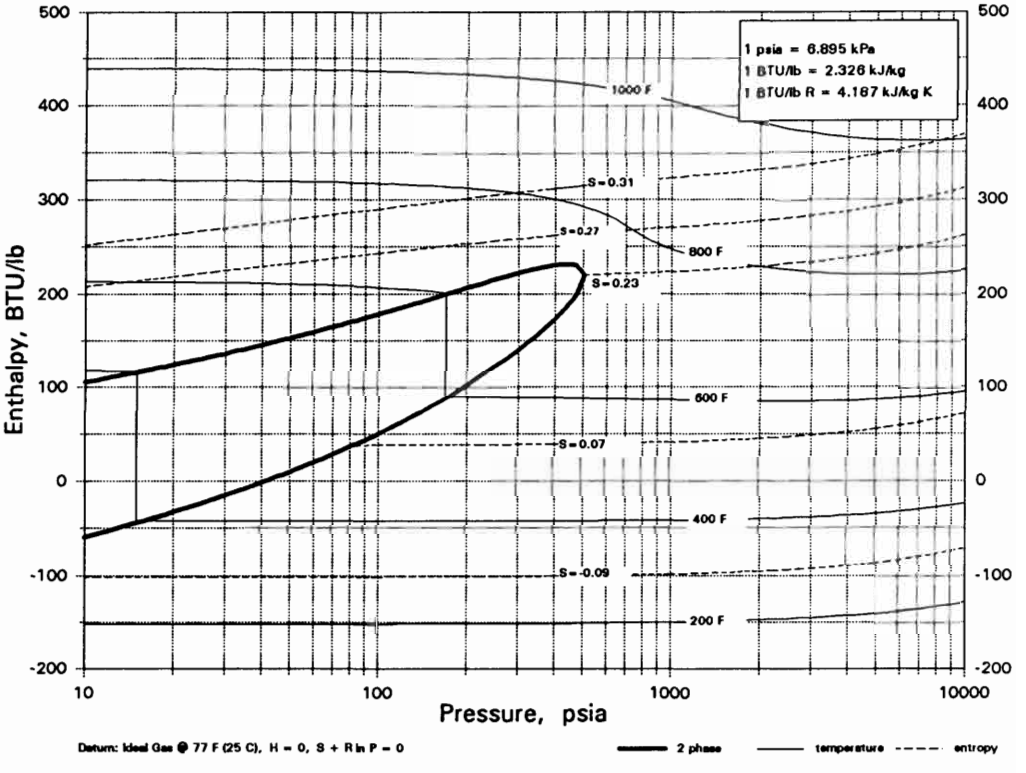
C9H12O BENZYL ETHYL ETHER



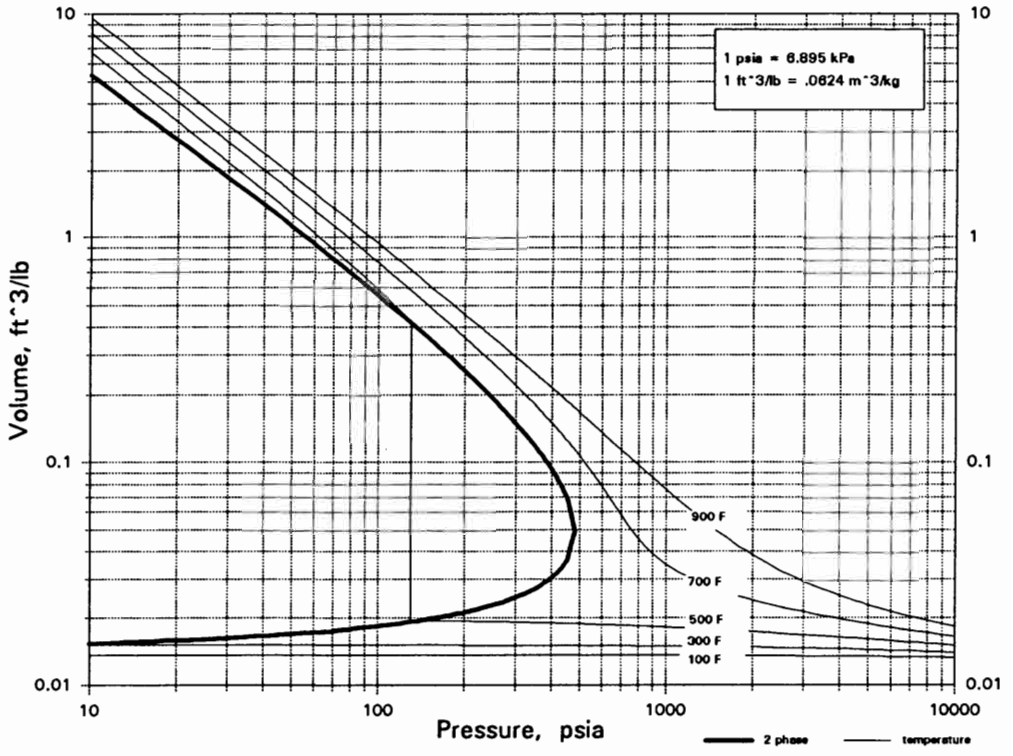


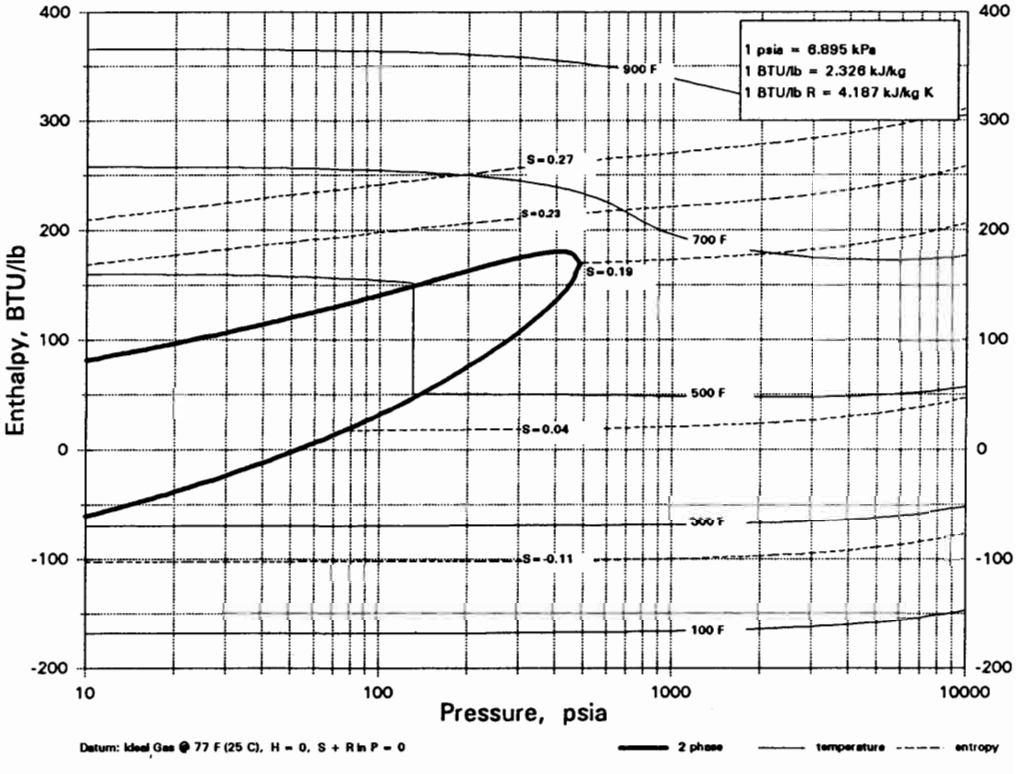
C9H12O 2-PHENYL-2-PROPANOL



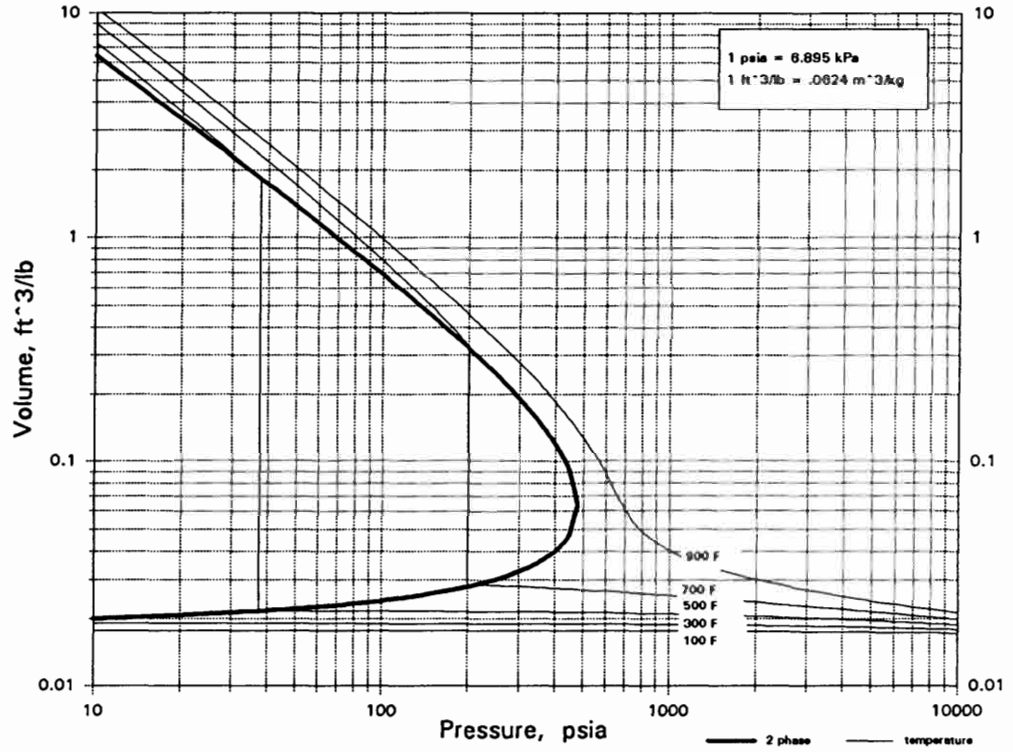


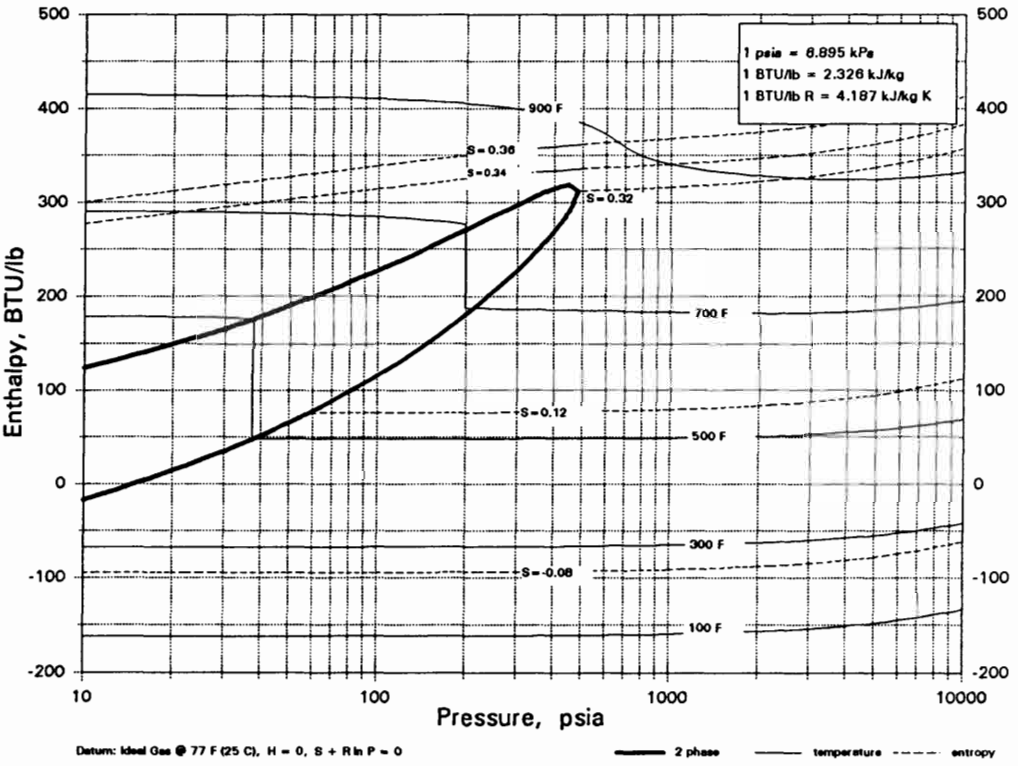
C9H12O2 CUMENE HYDROPEROXIDE



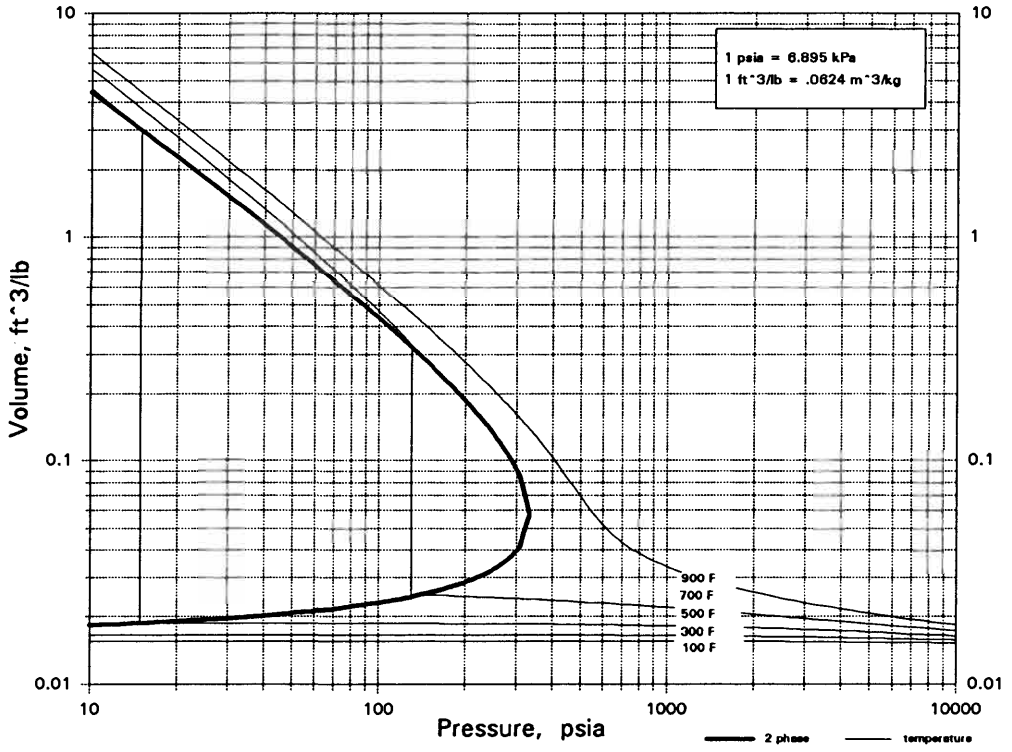


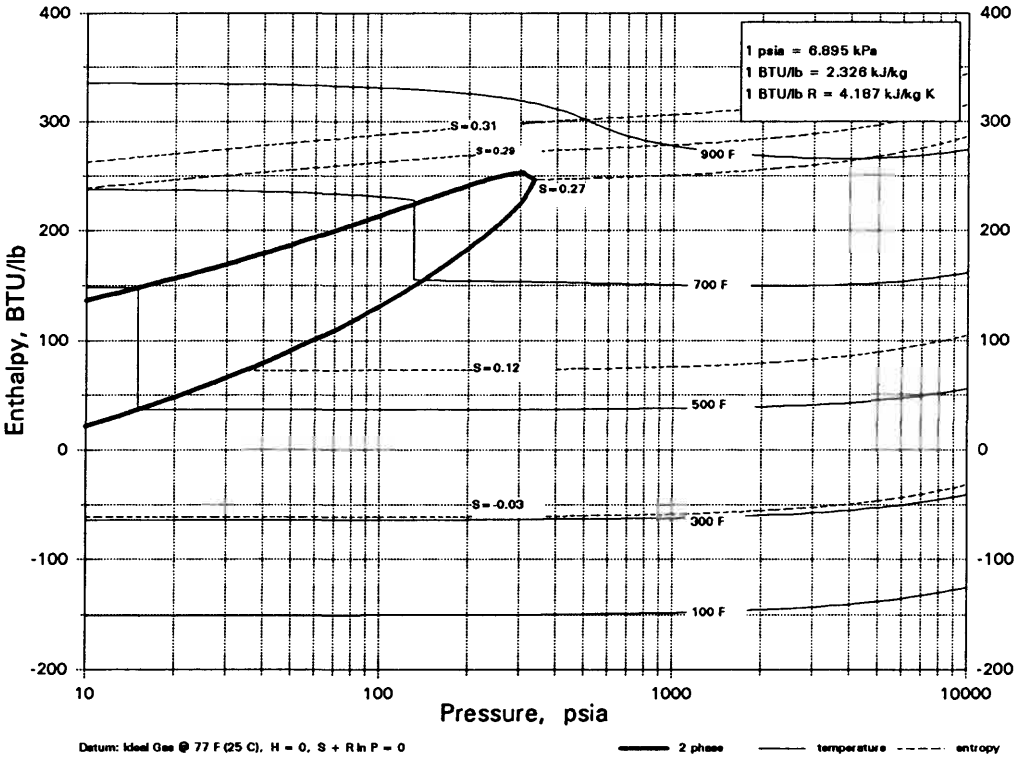
C9H14O ISOPHORONE



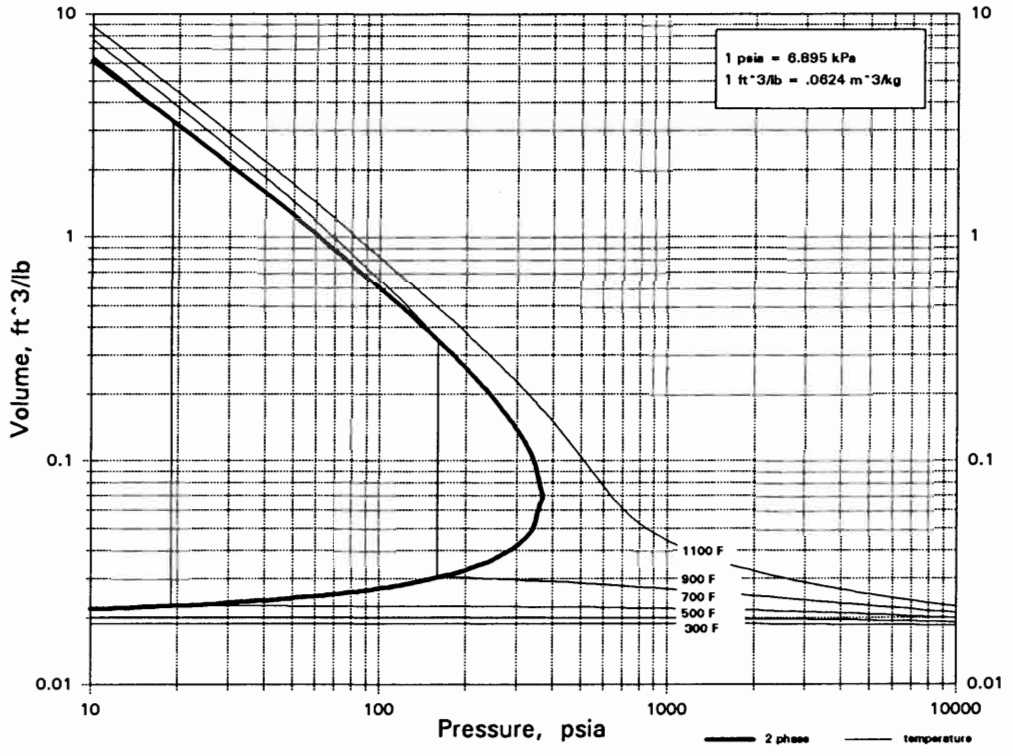


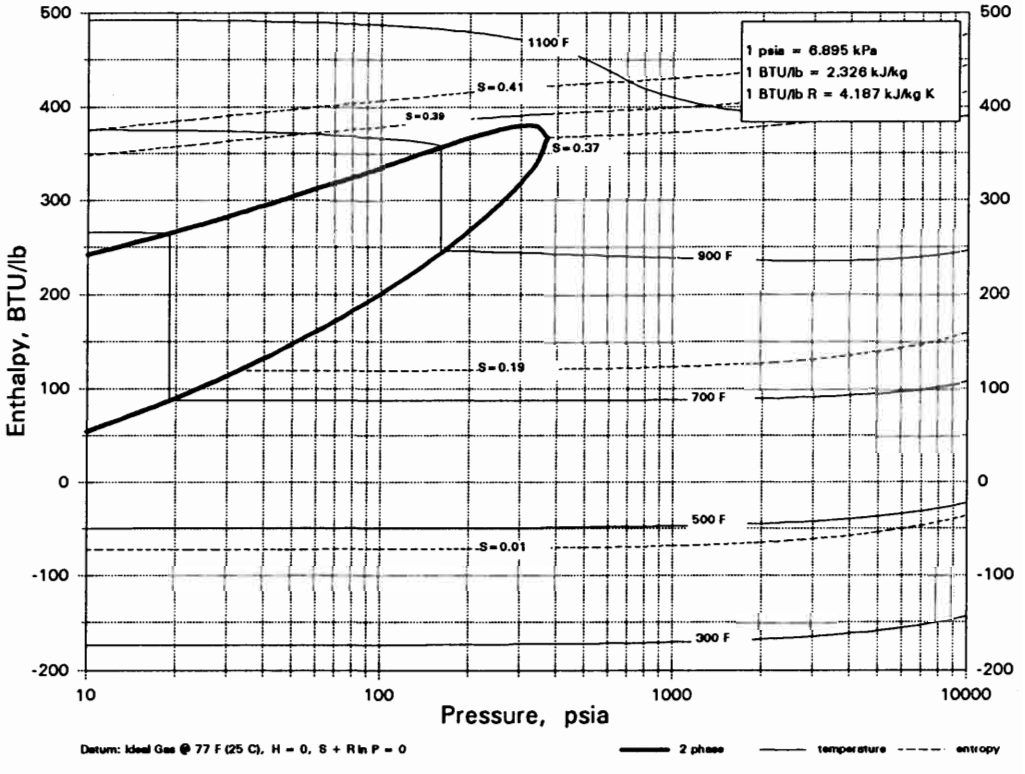
C9H14O6 GLYCERYL TRIACETATE



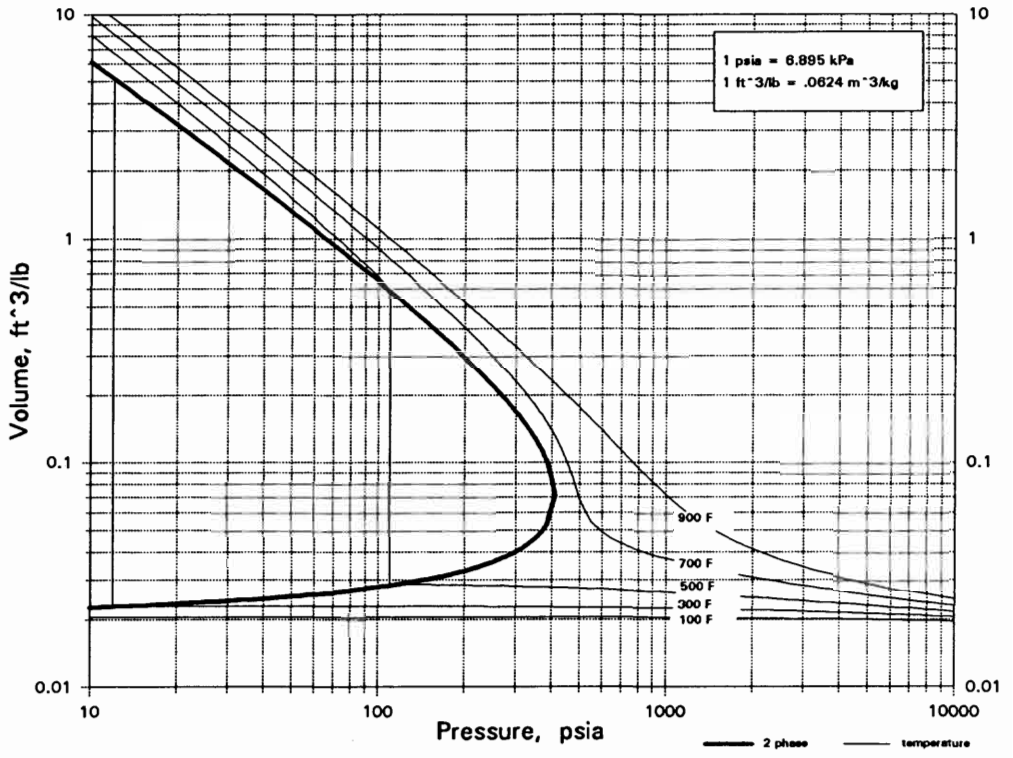


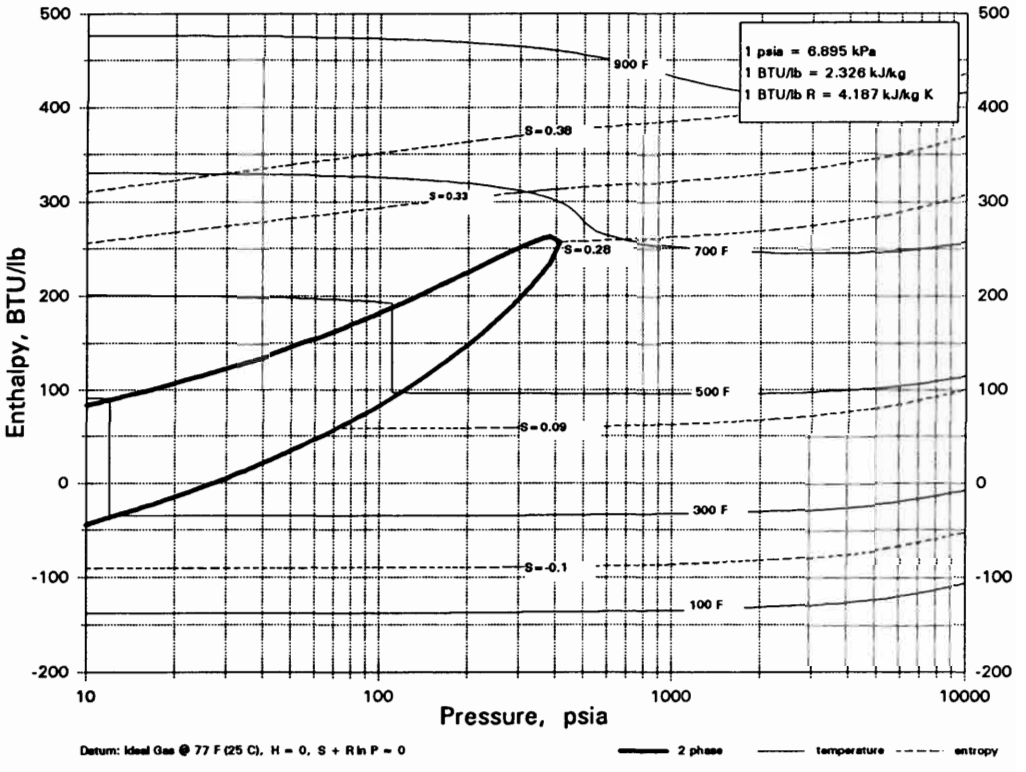
C9H16O4 AZELAIC ACID



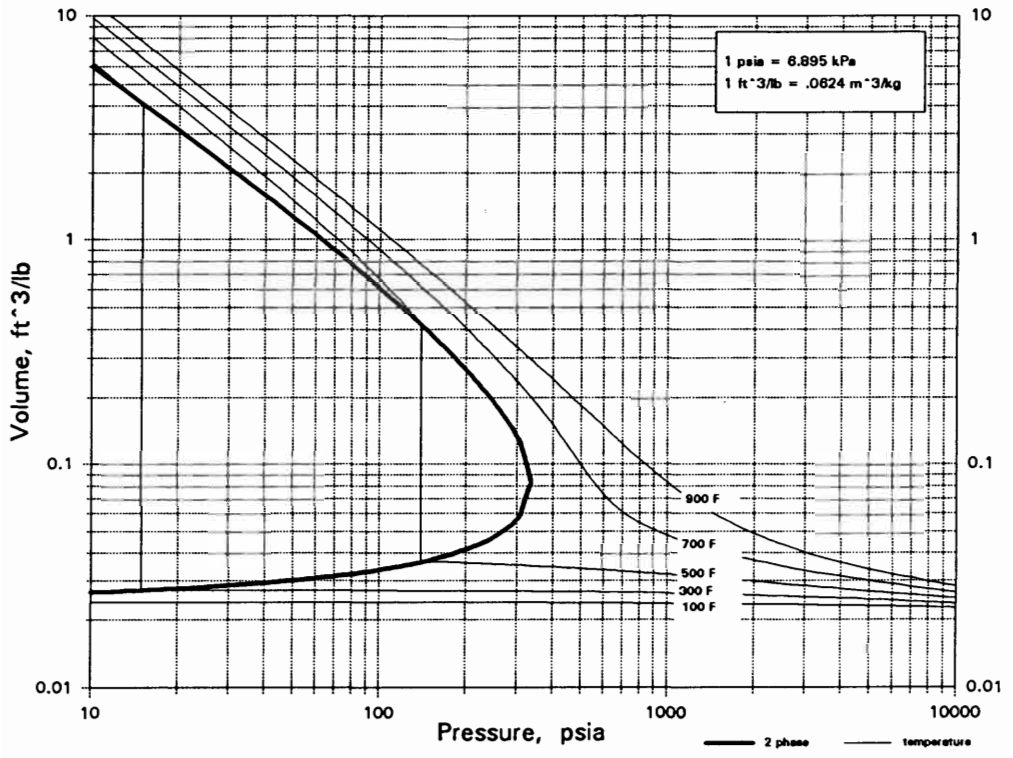


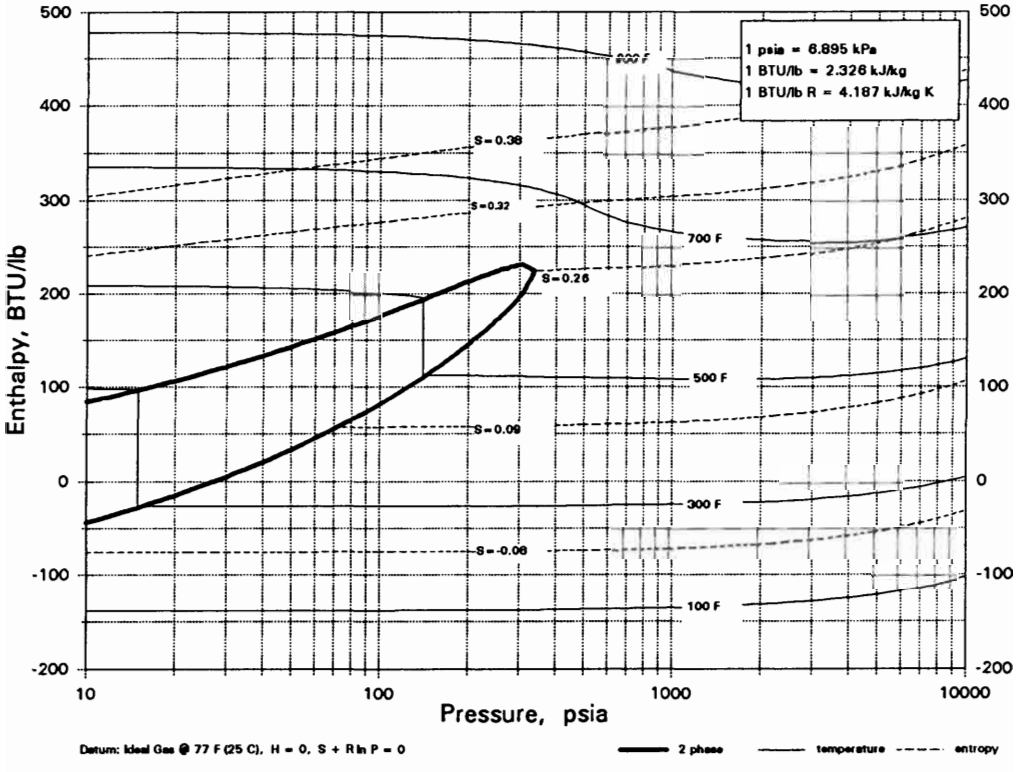
C9H18 ISOPROPYLCYCLOHEXANE



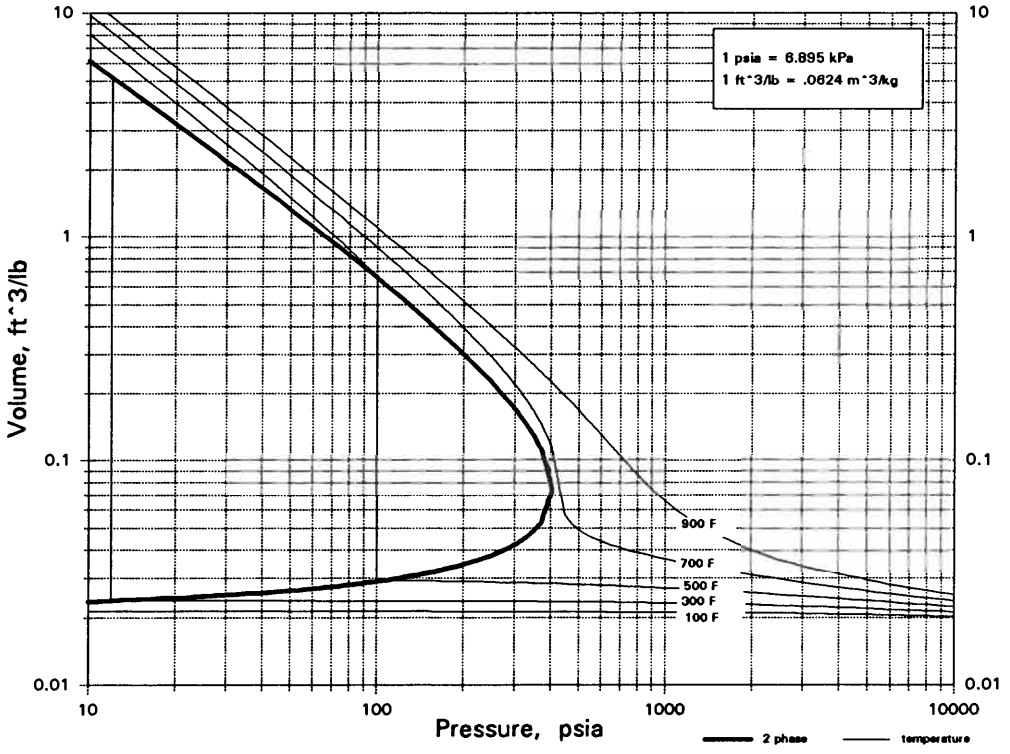


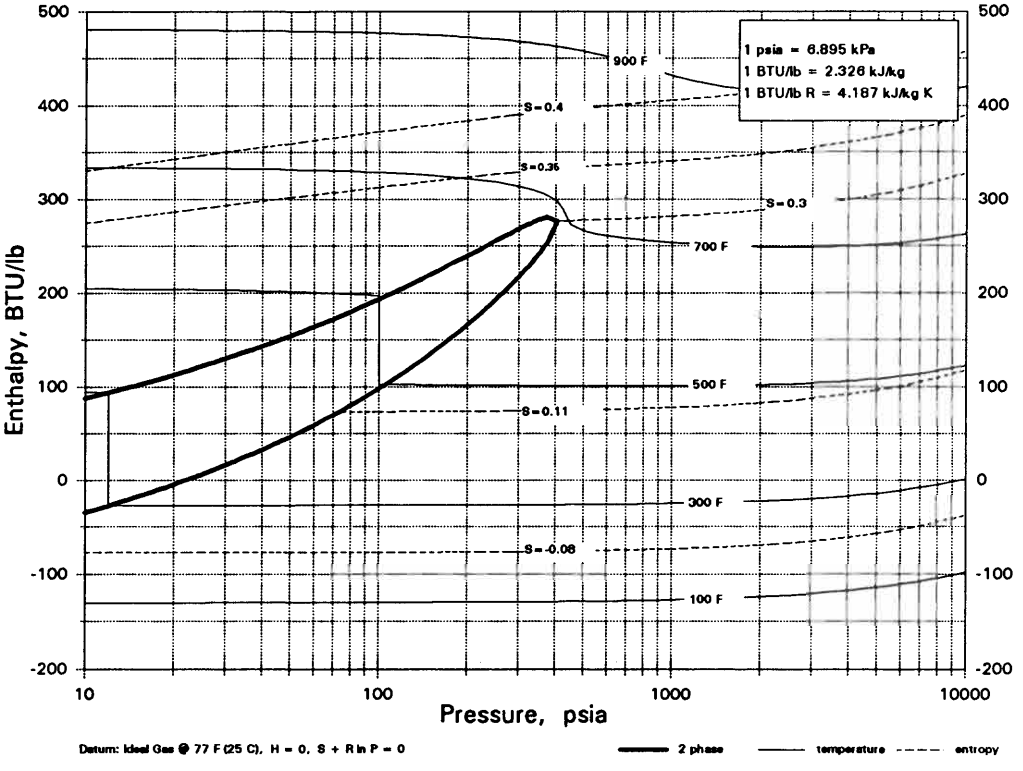
C9H18 1-NONENE



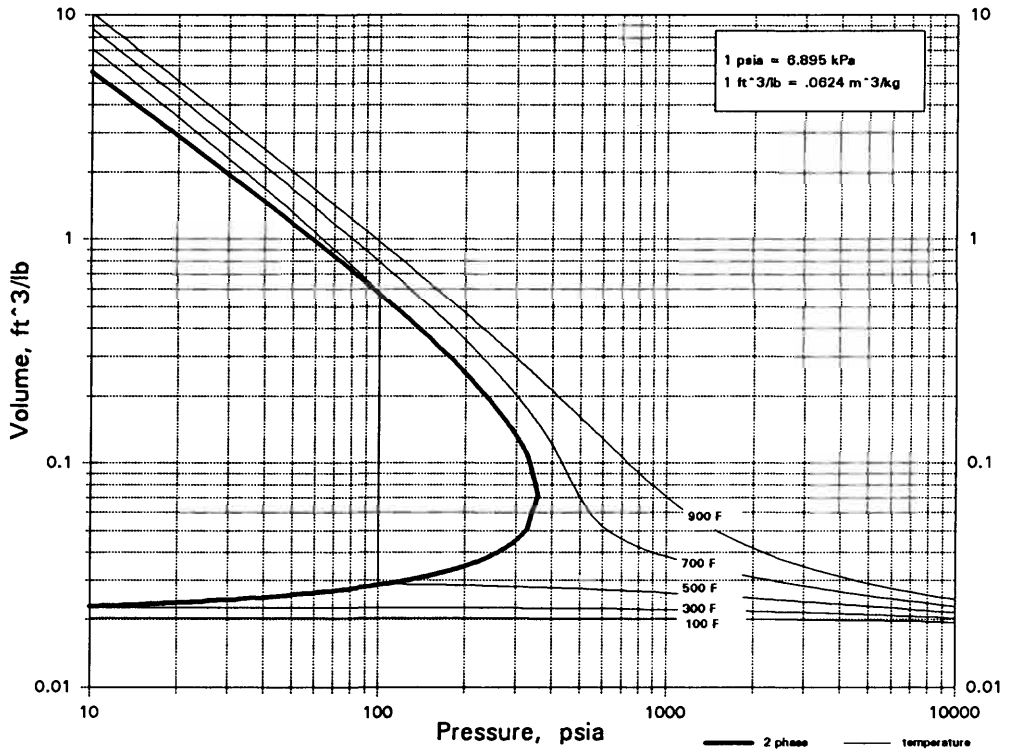


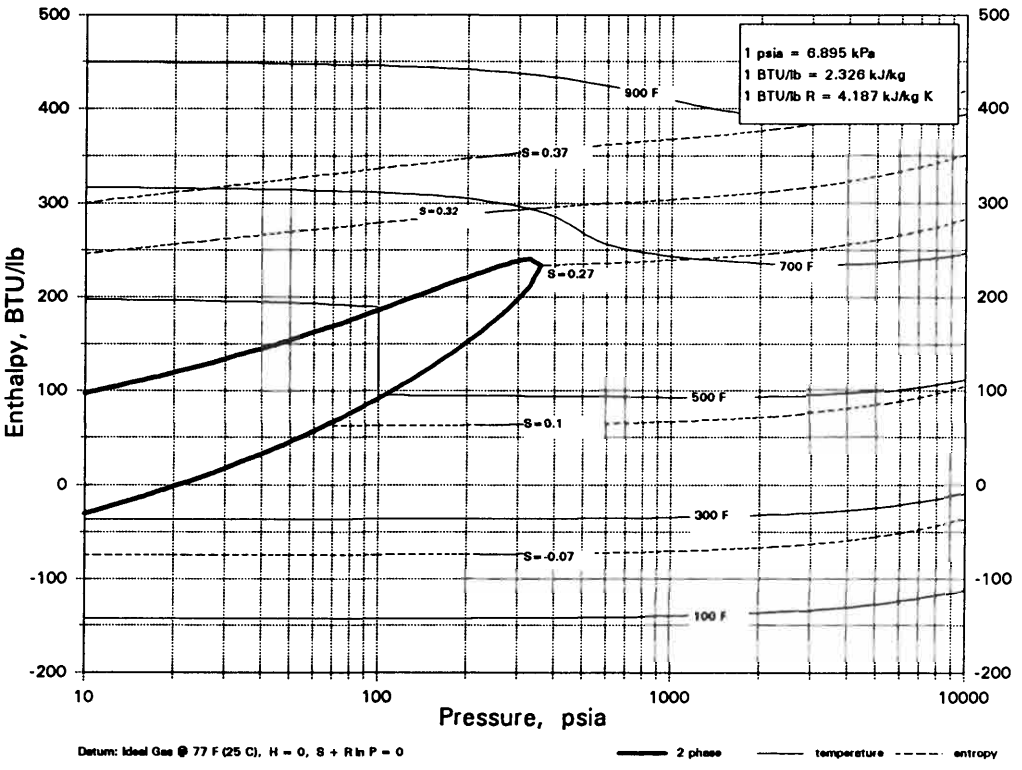
C9H18 n-PROPYLCYCLOHEXANE



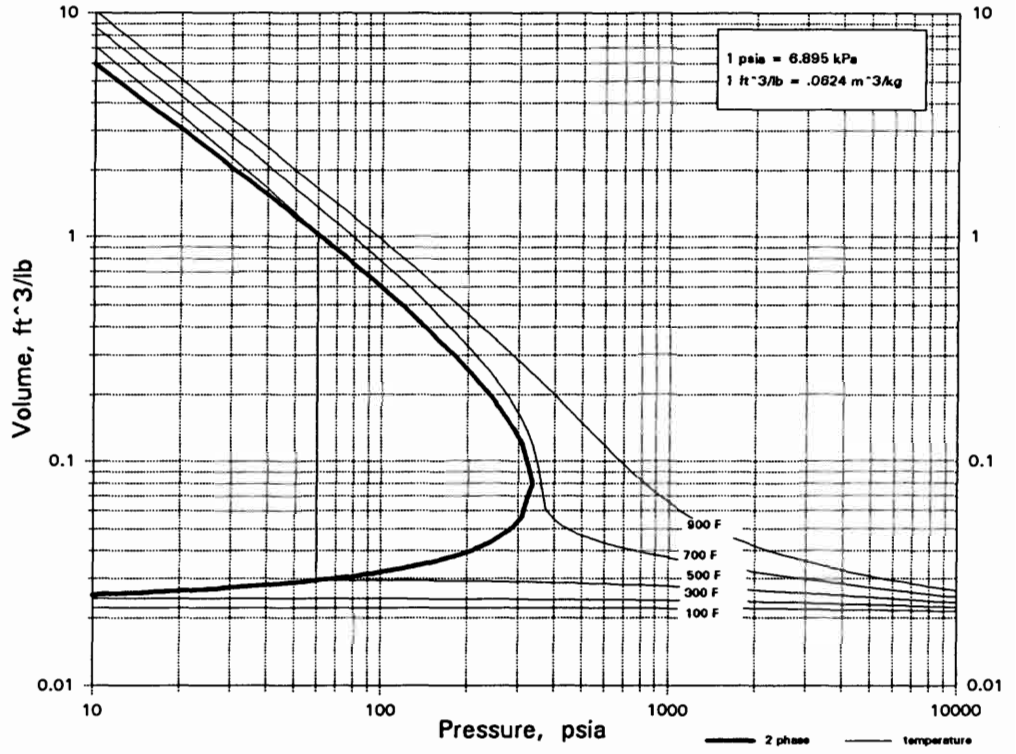


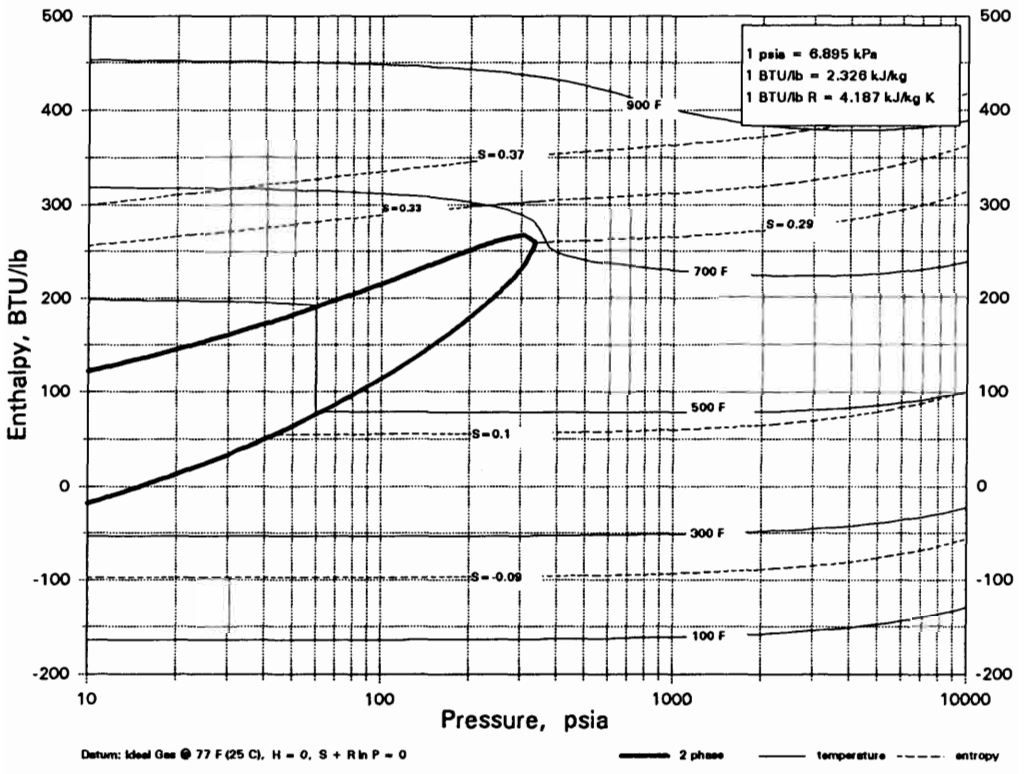
C9H18O DIISOBUTYL KETONE



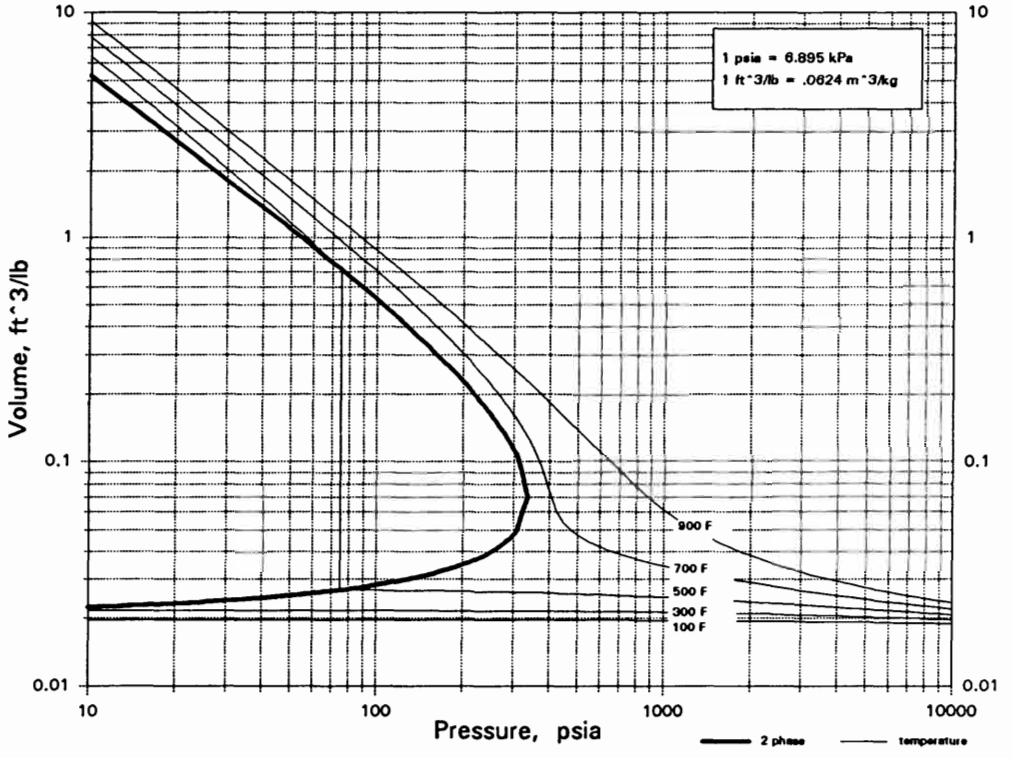


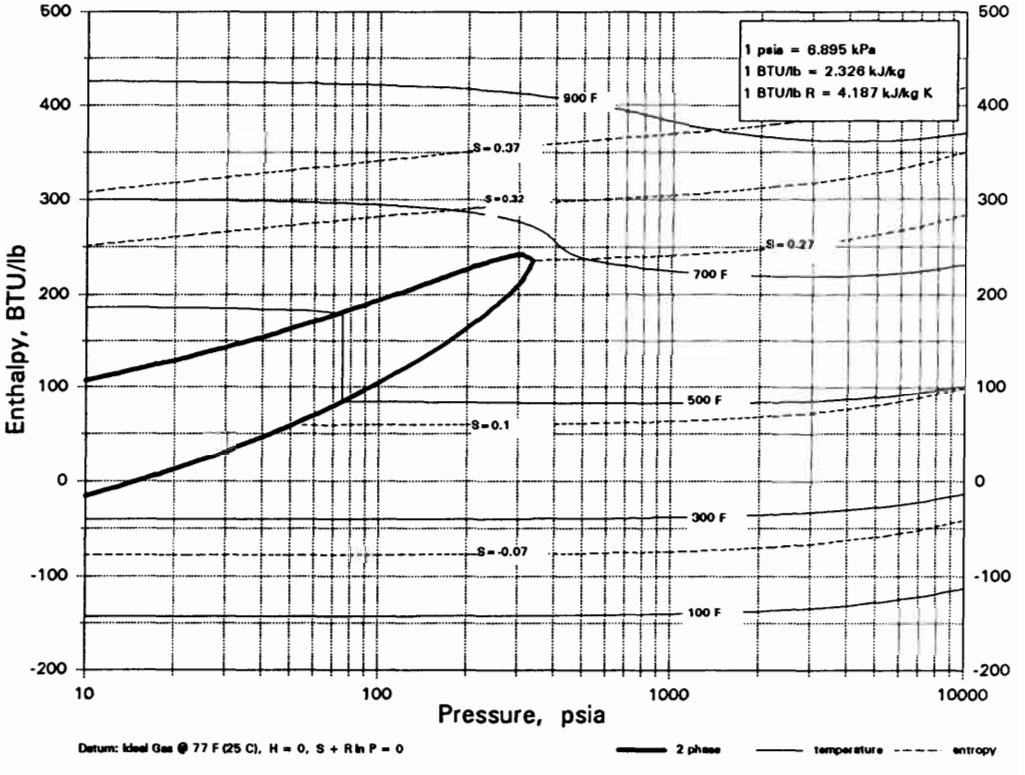
C9H18O 1-NONANAL



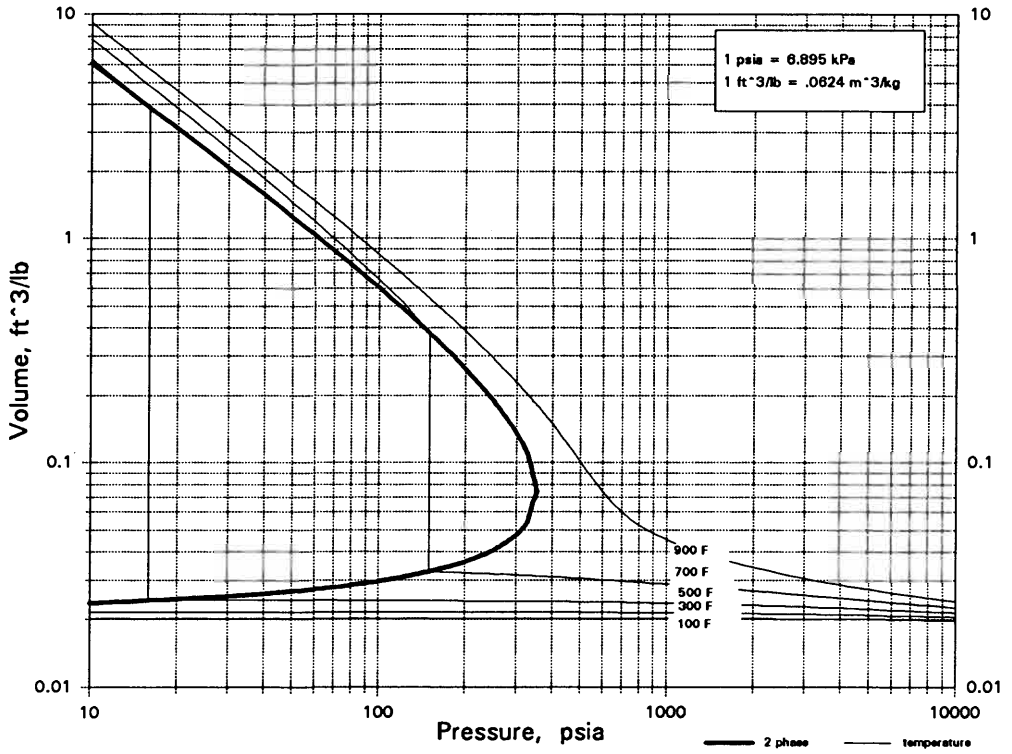


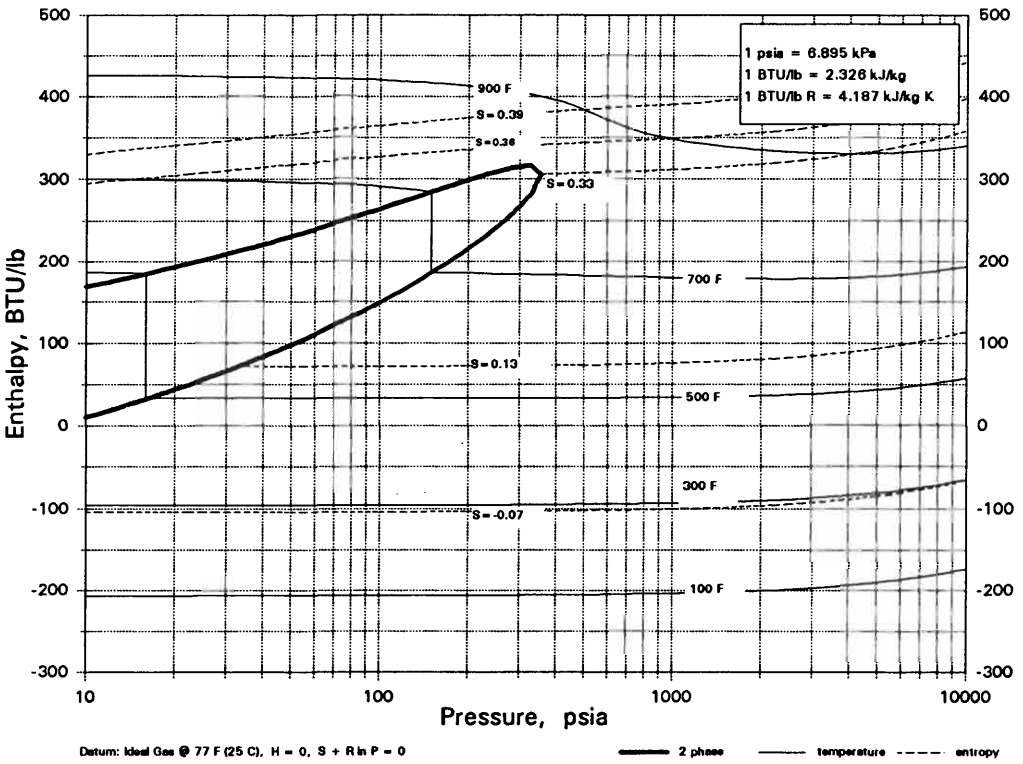
C9H18O2 n-BUTYL VALERATE



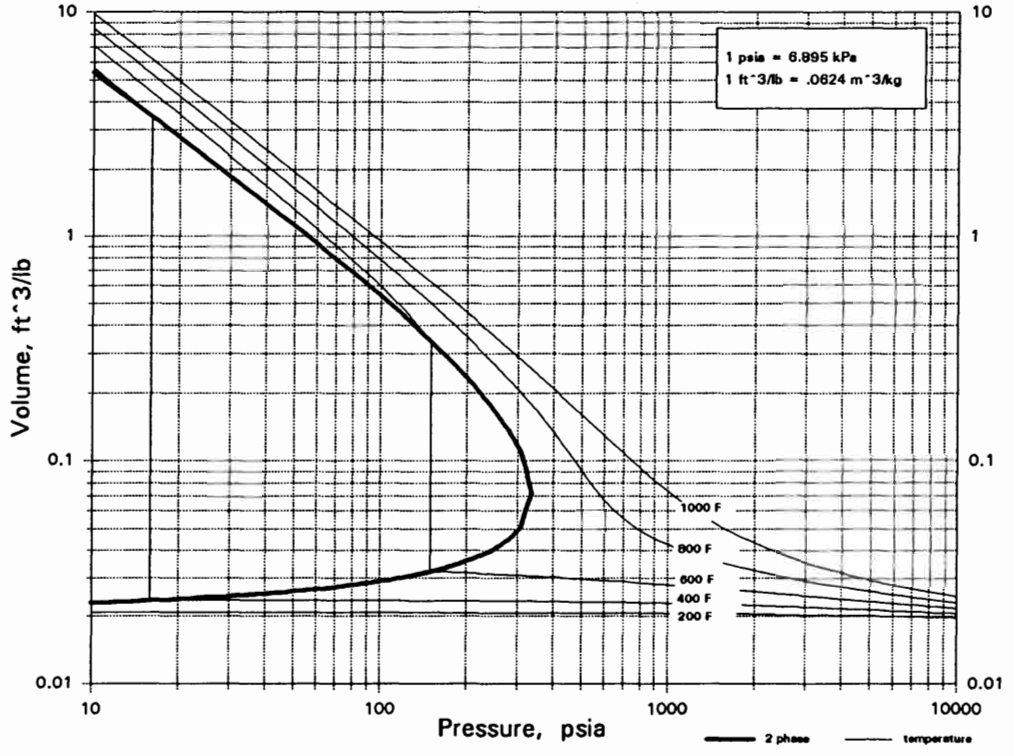


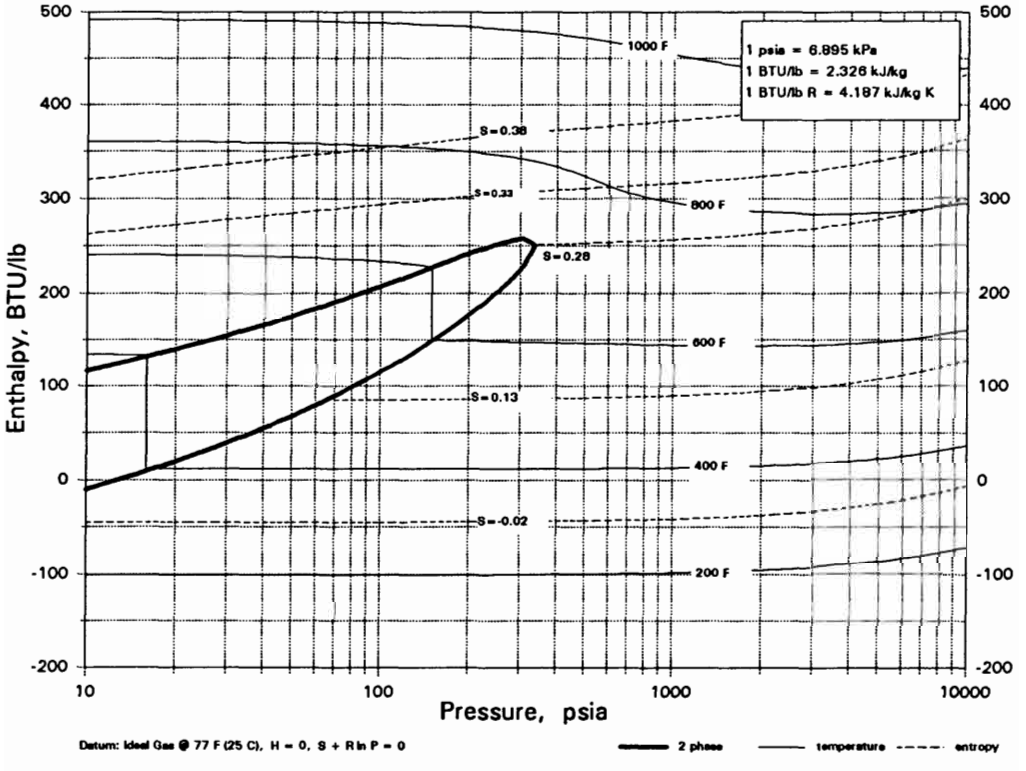
C9H18O2 n-NONANOIC ACID



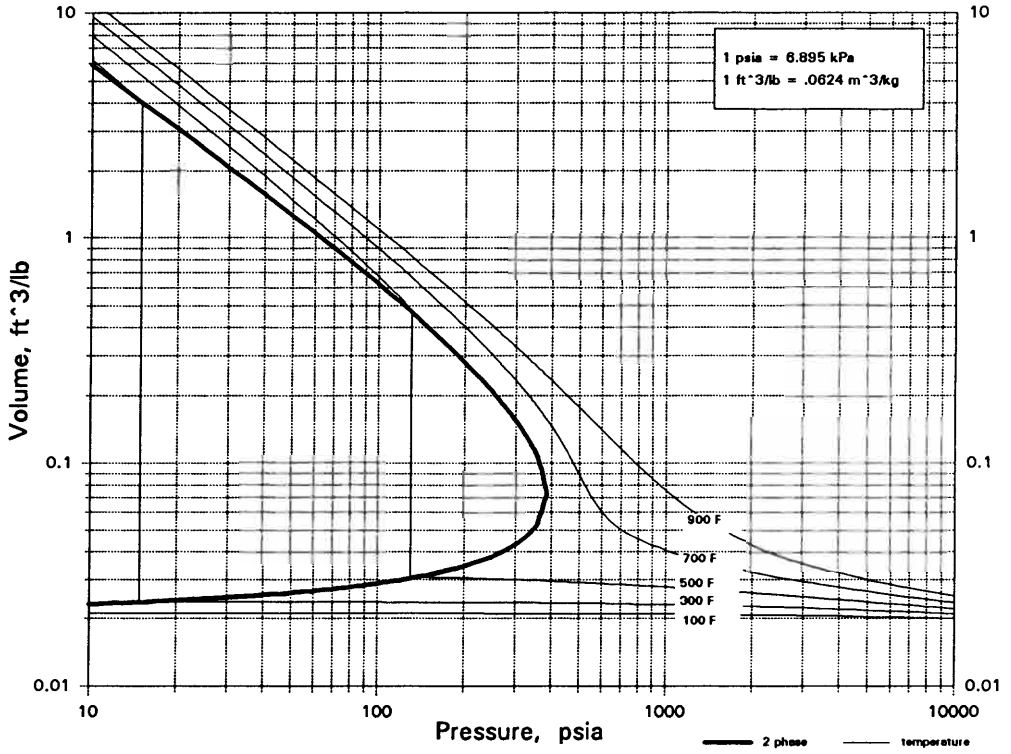


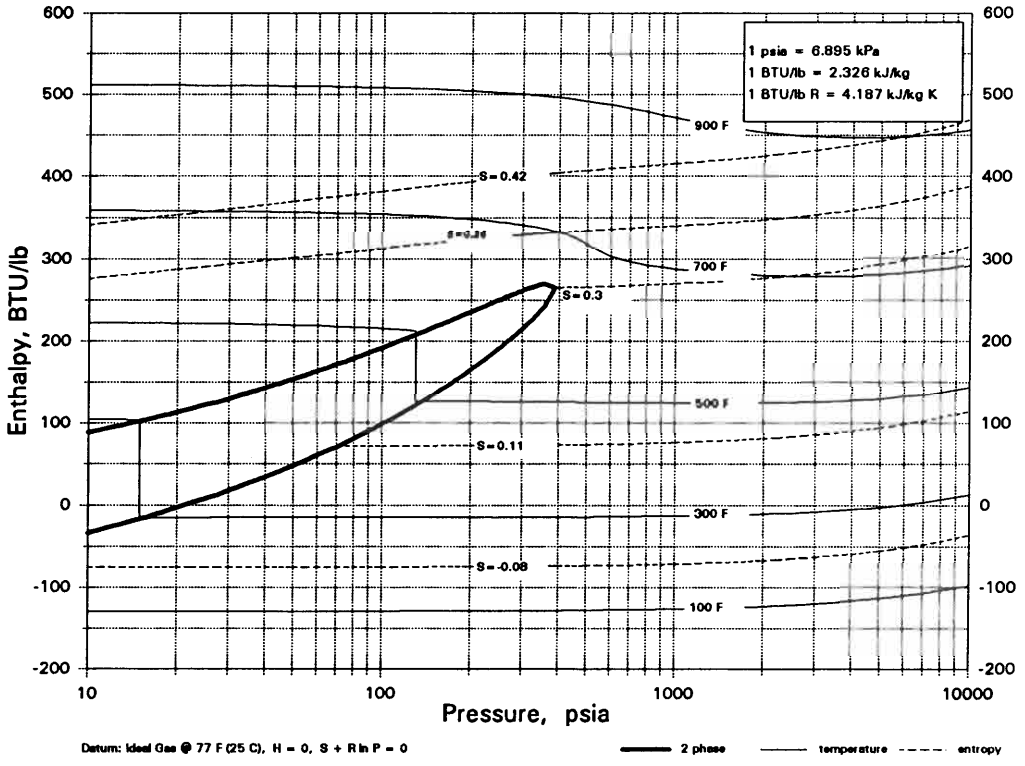
C9H18O2 n-OCTYL FORMATE



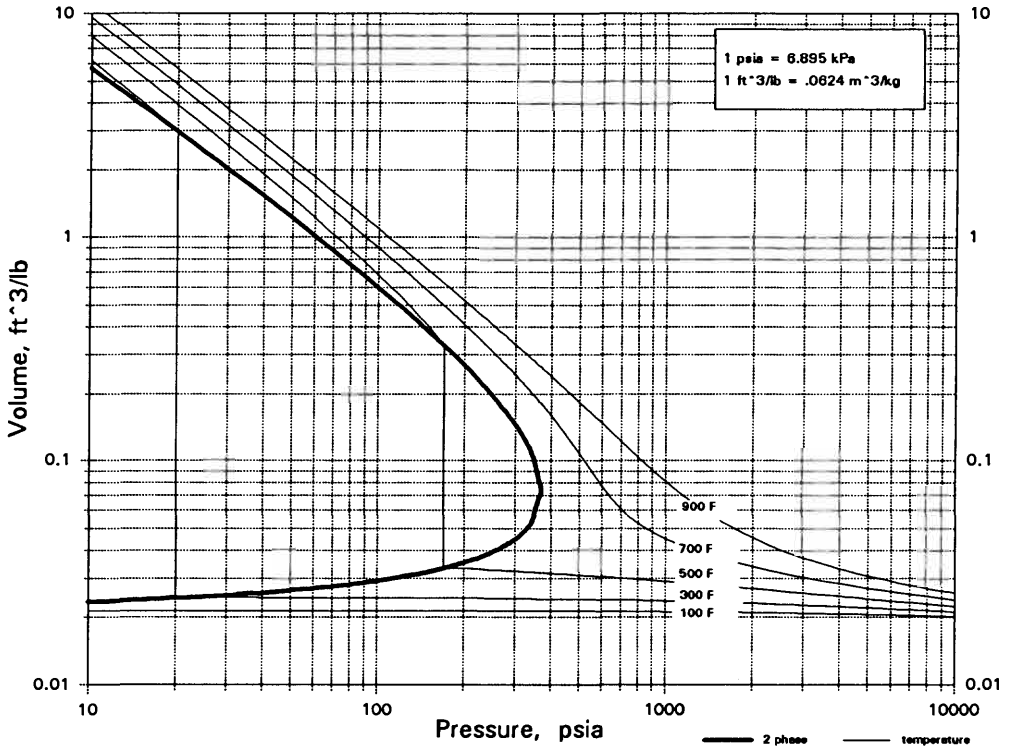


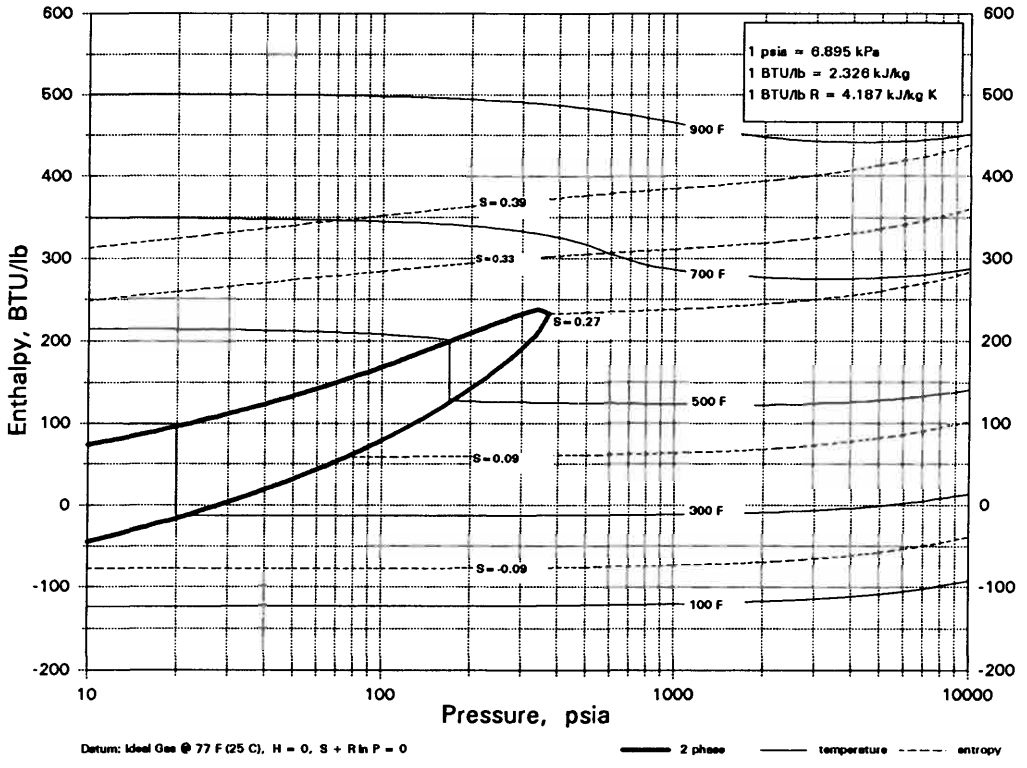
C9H20 3-3-DIETHYLPENTANE



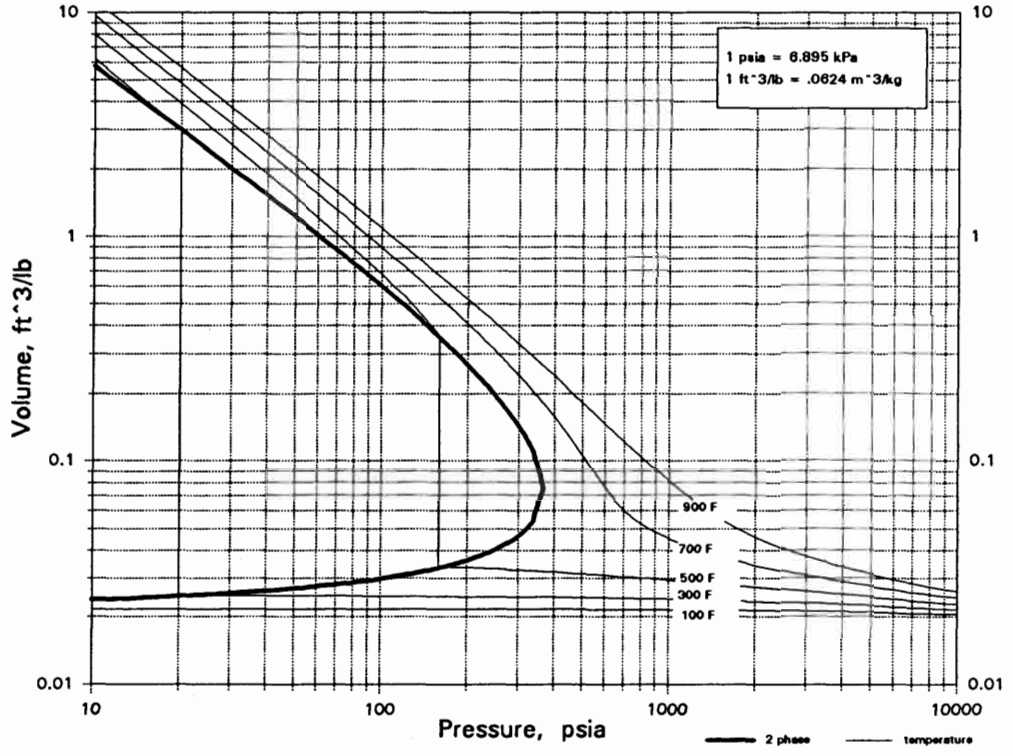


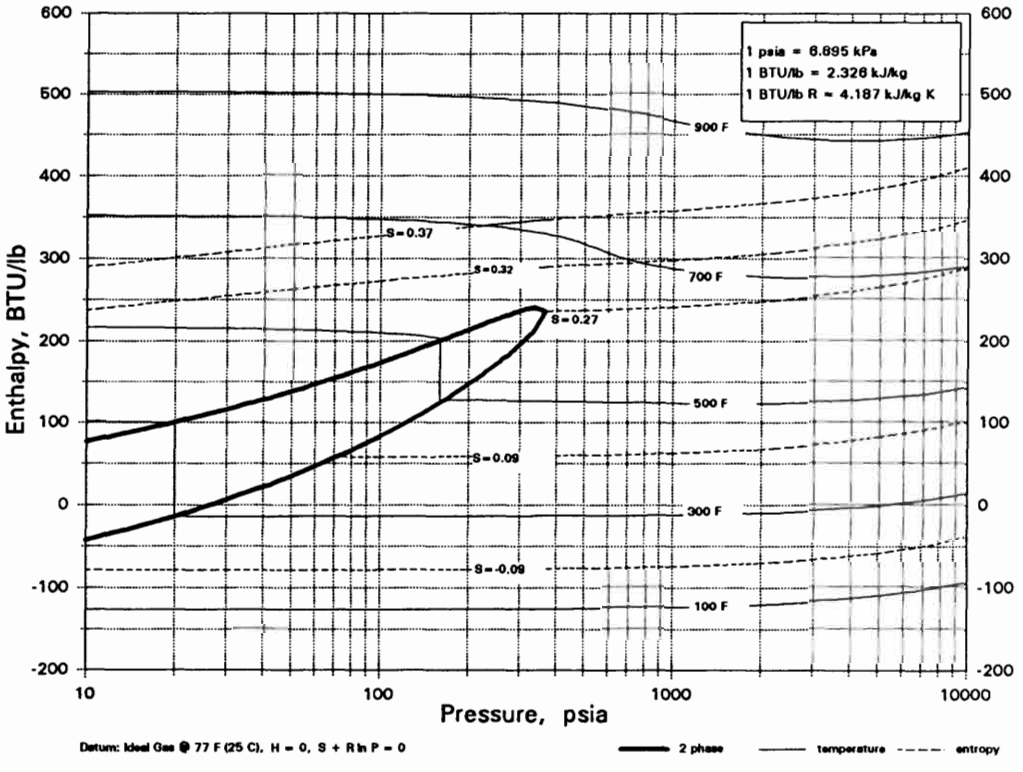
C9H20	2-2-DIMETHYL-3-ETHYLPENTANE



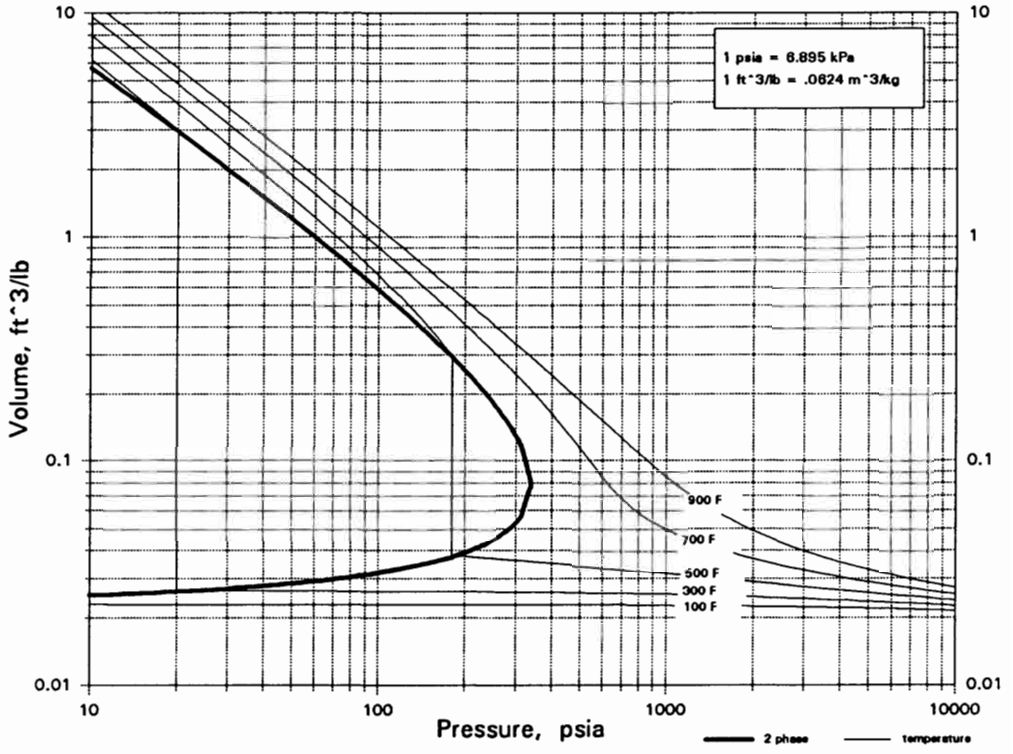


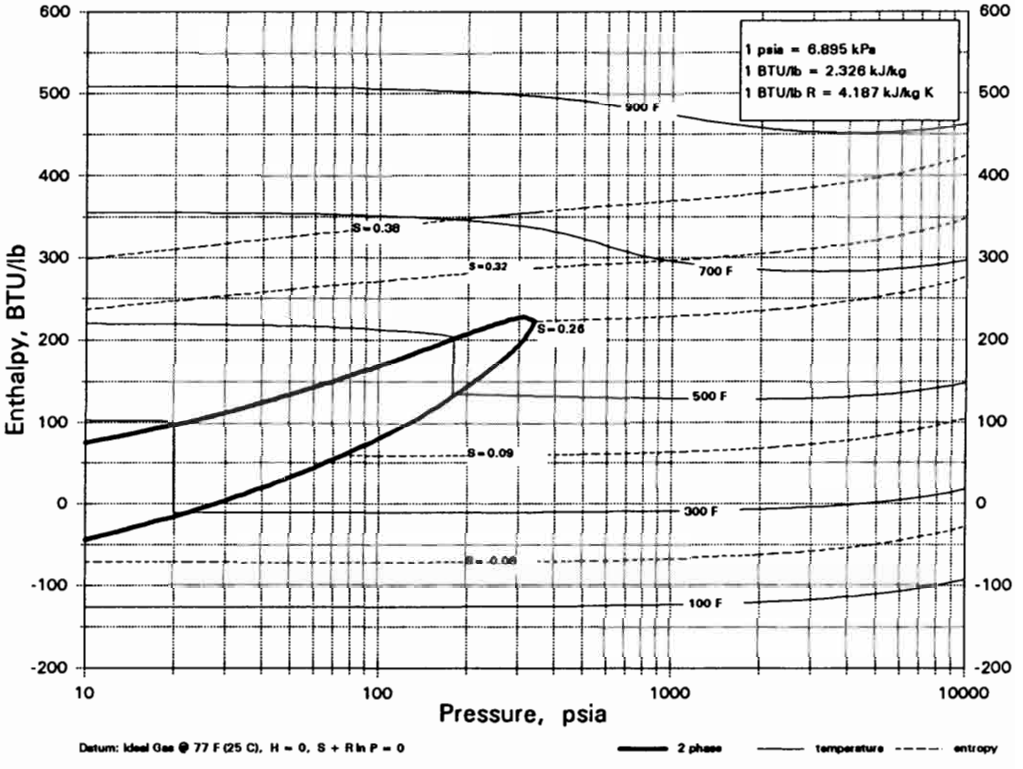
C9H20 2-4-DIMETHYL-3-ETHYLPENTANE



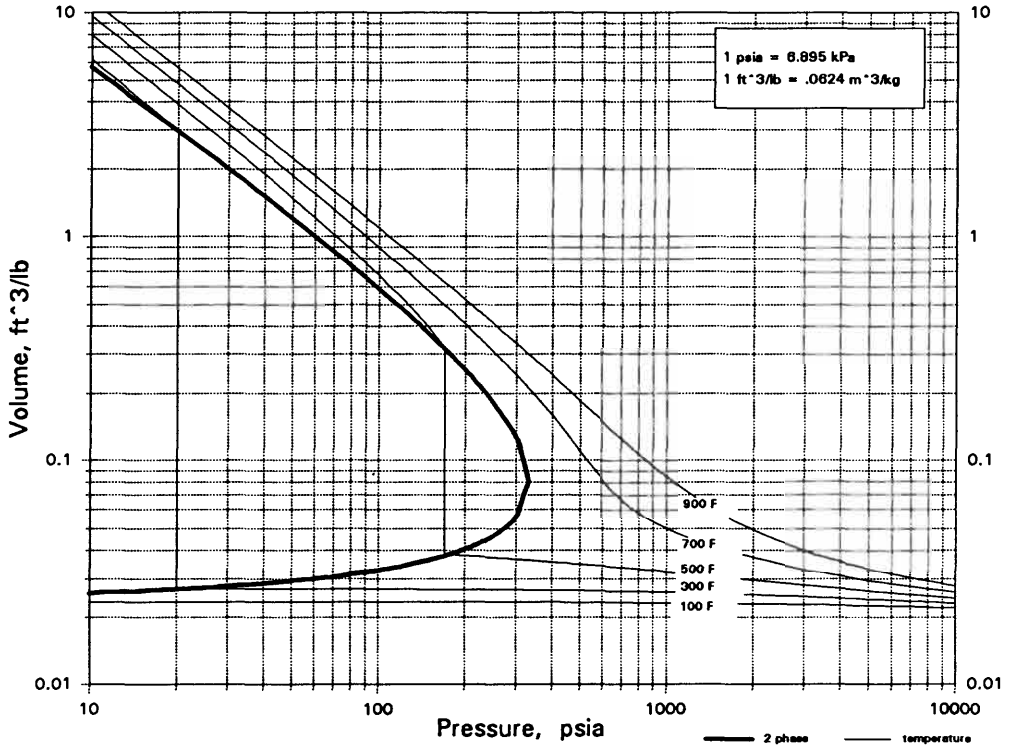


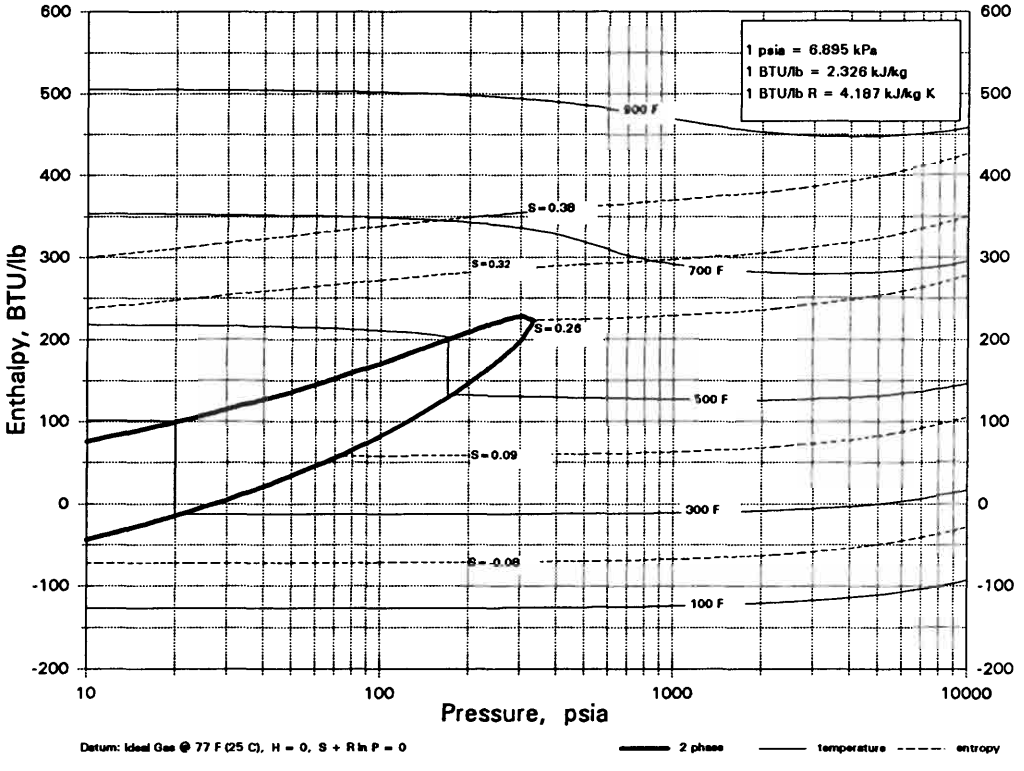
C9H20 2-2-DIMETHYLHEPTANE



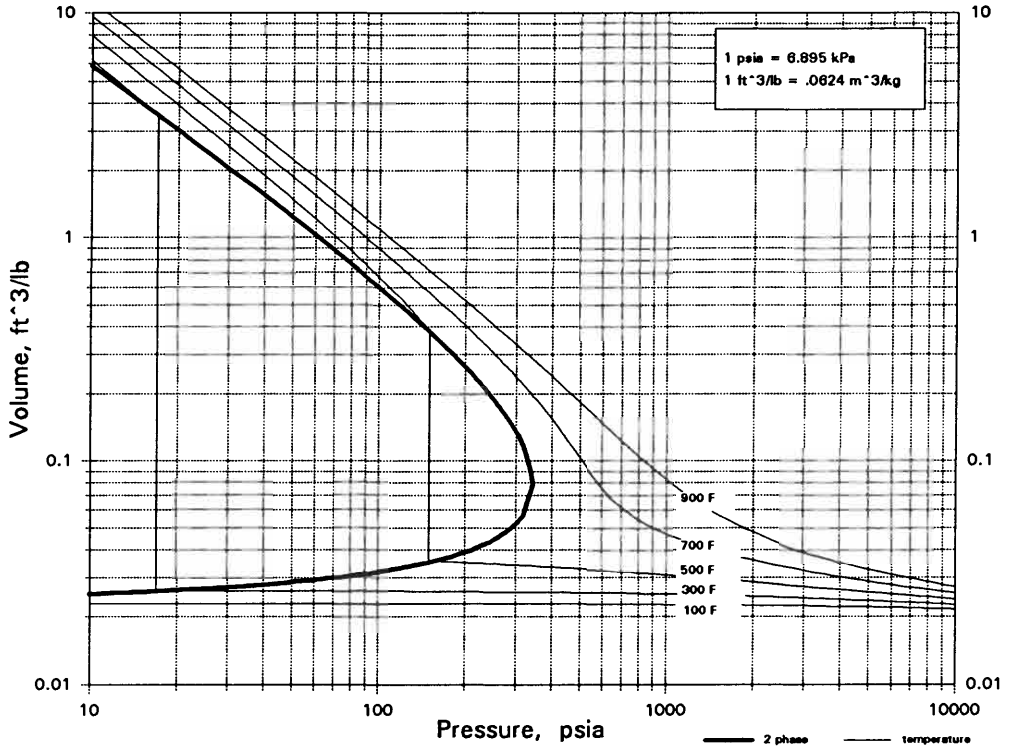


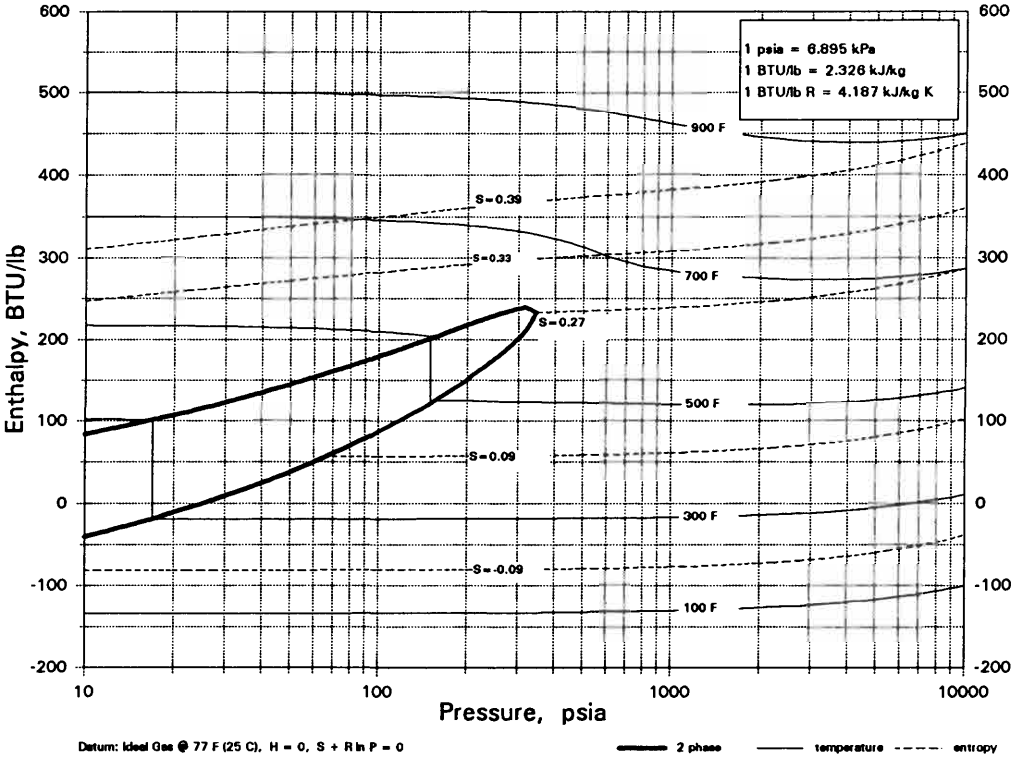
C9H20 2-6-DIMETHYLHEPTANE



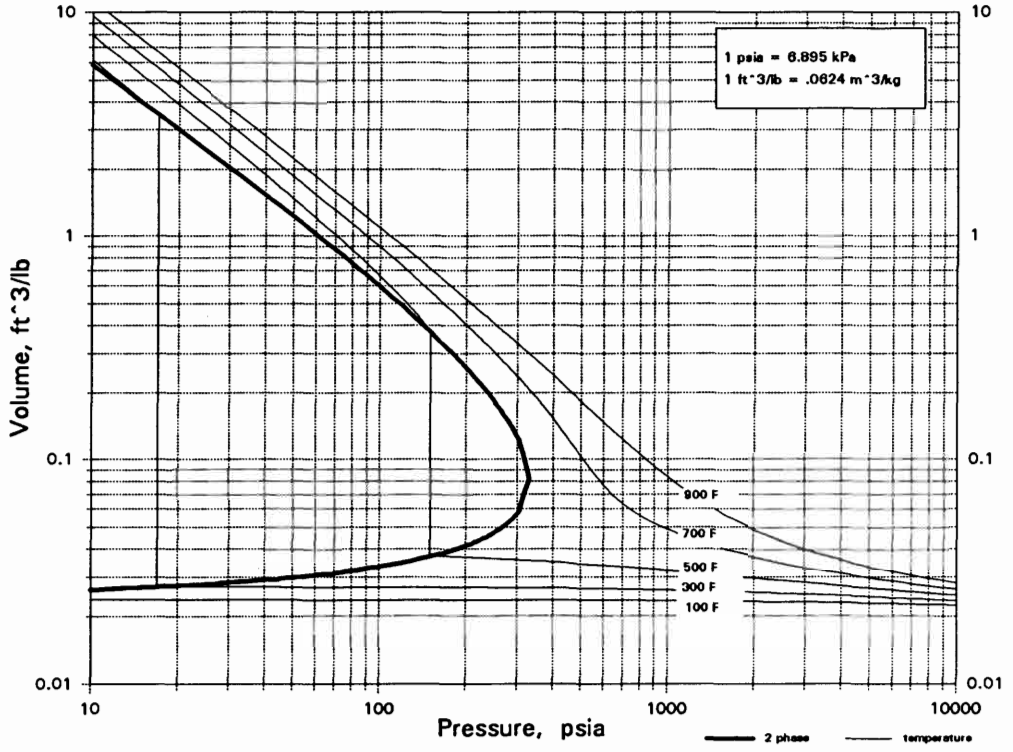


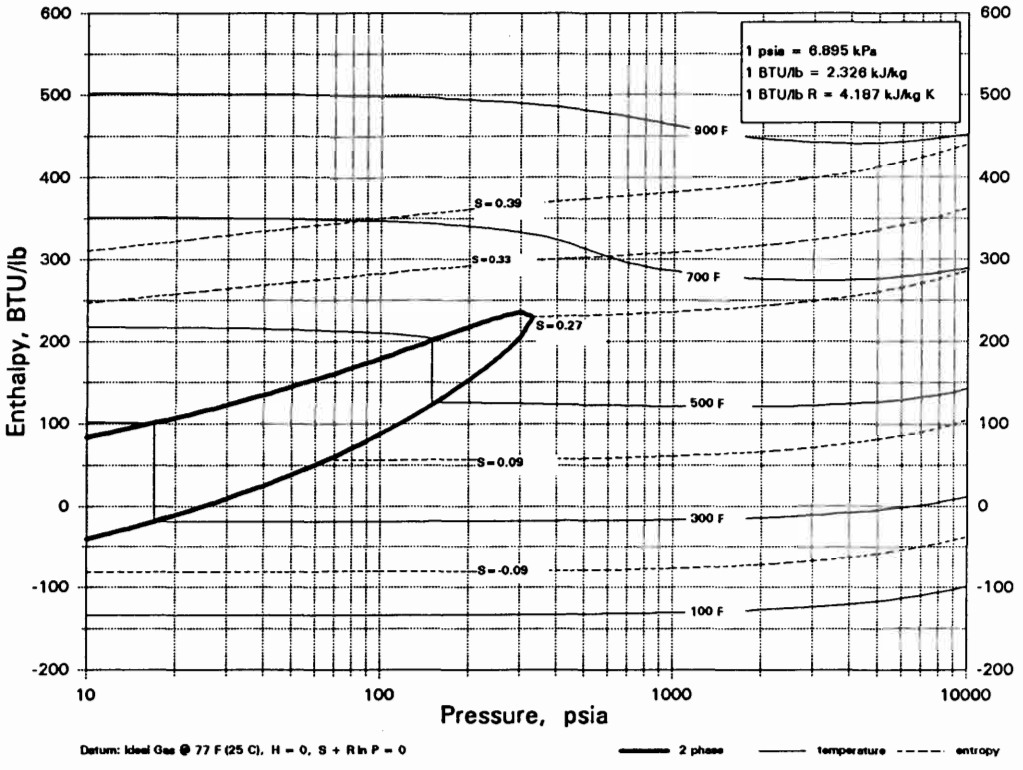
C9H20 3-ETHYLHEPTANE



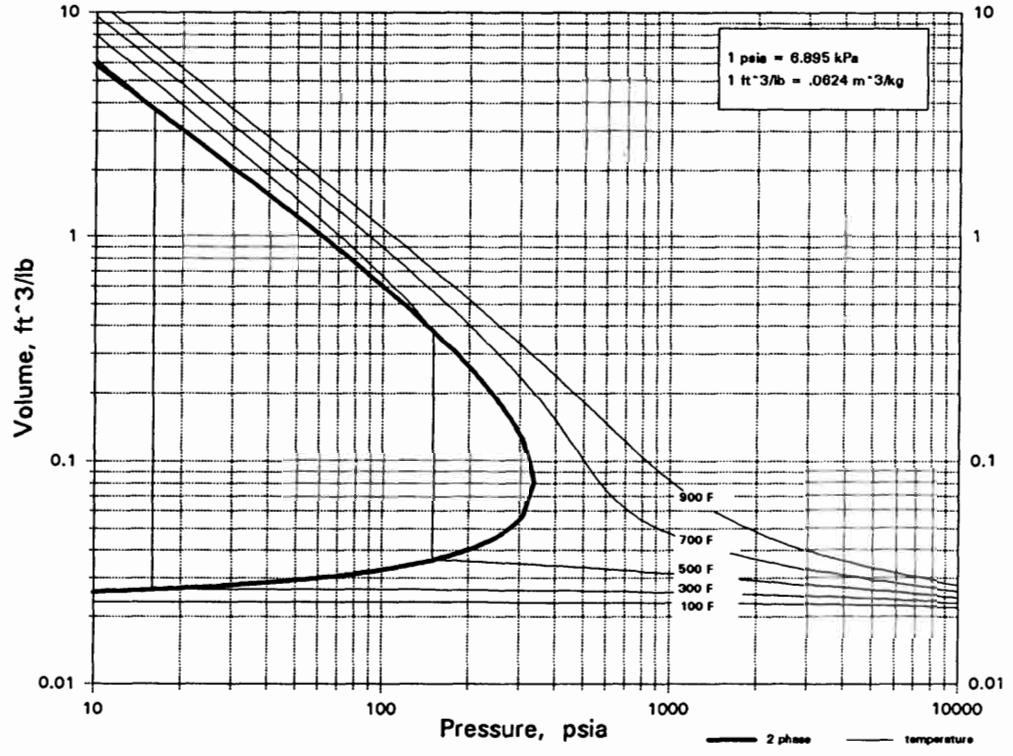


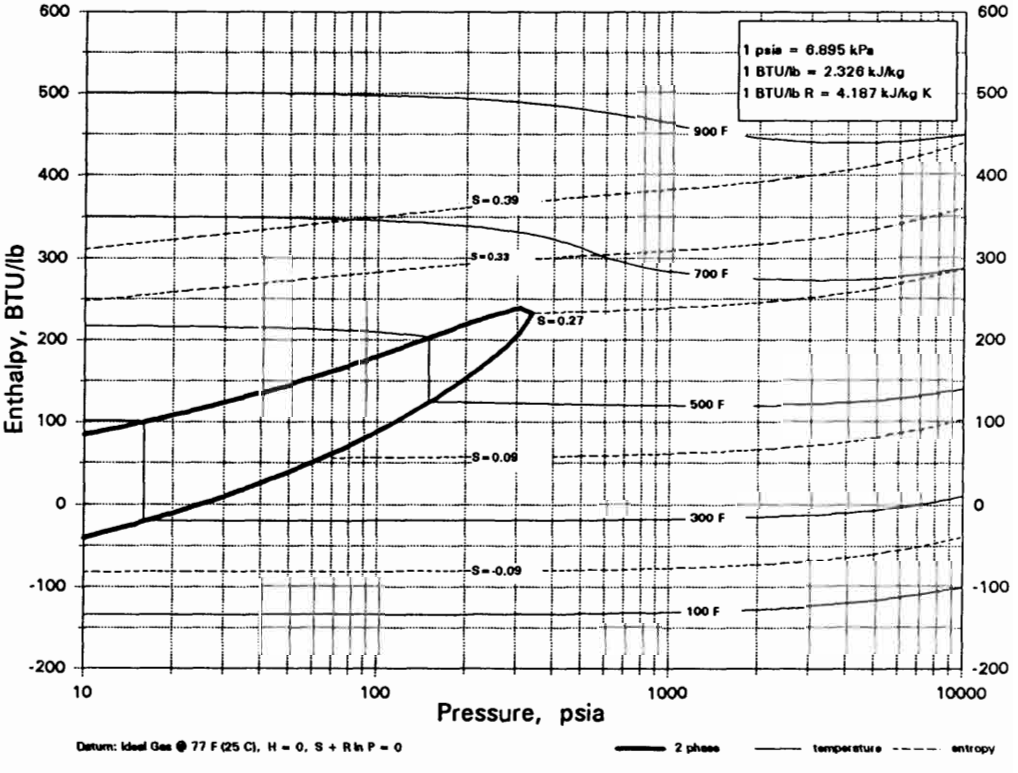
C9H20 2-METHYLOCTANE



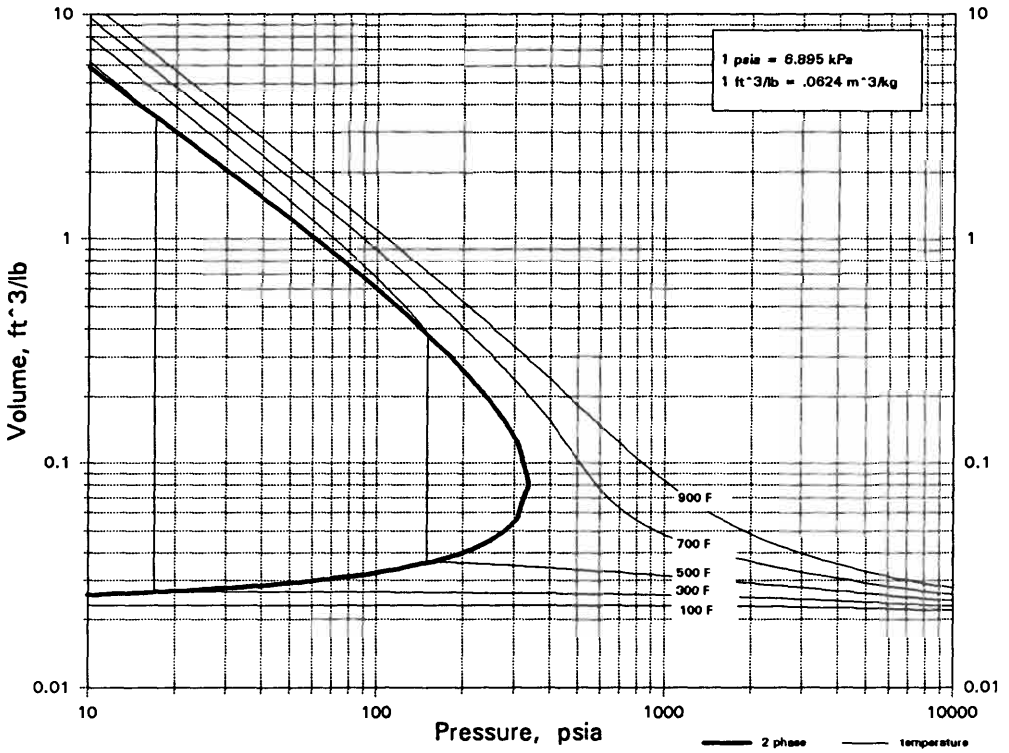


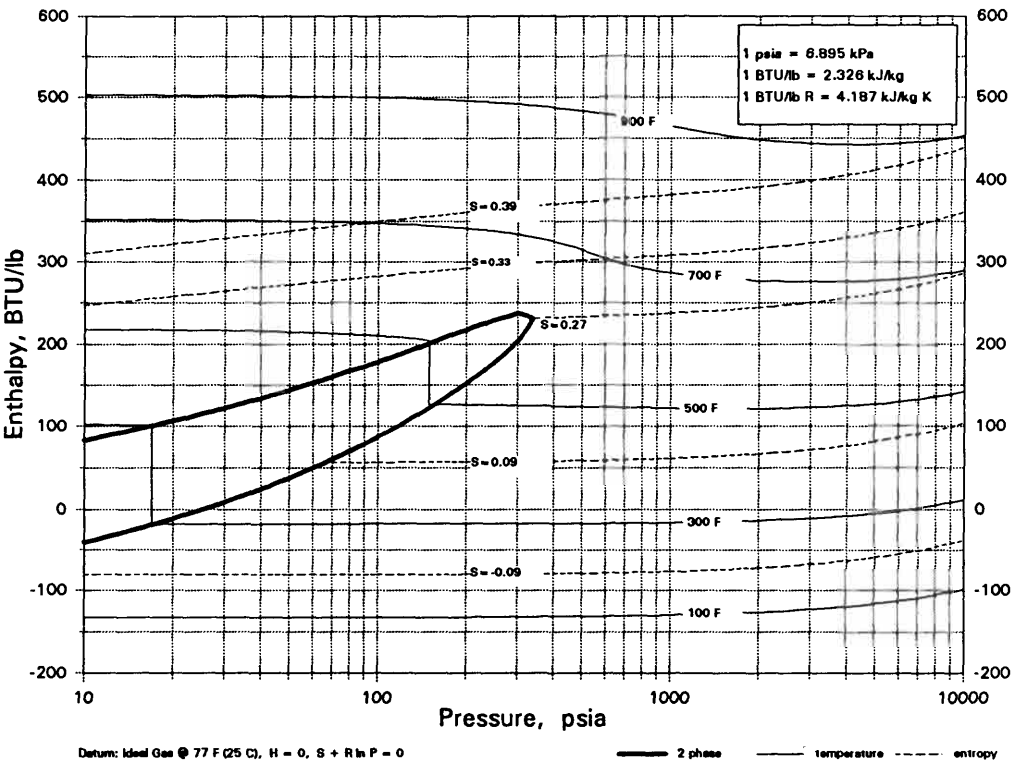
C9H20 3-METHYLOCTANE



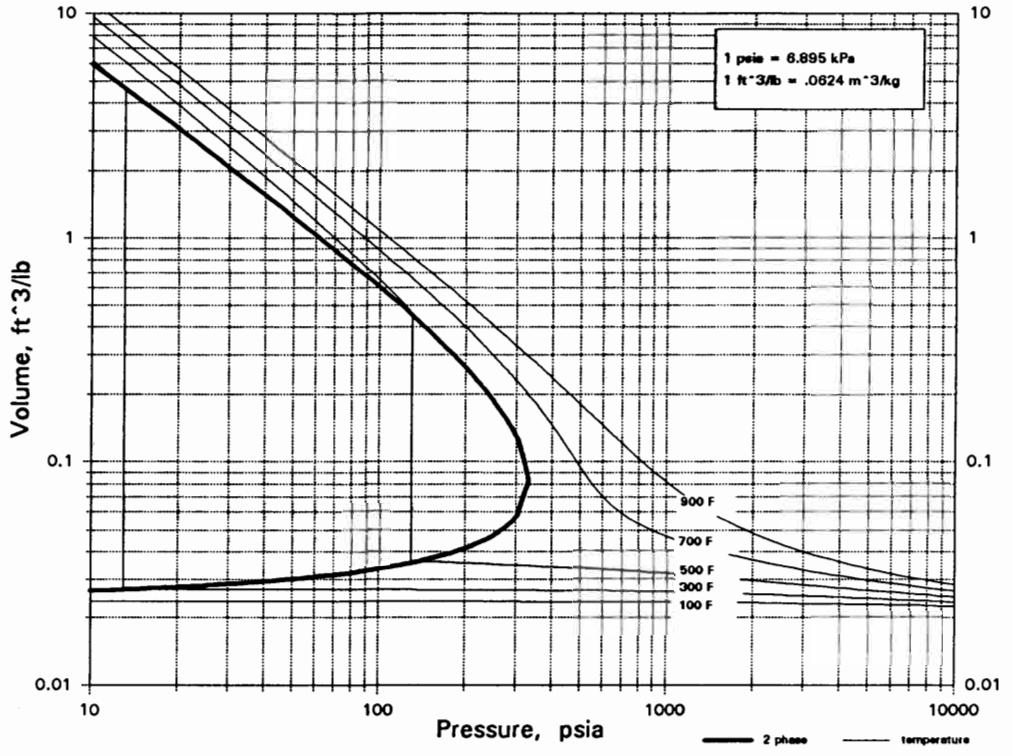


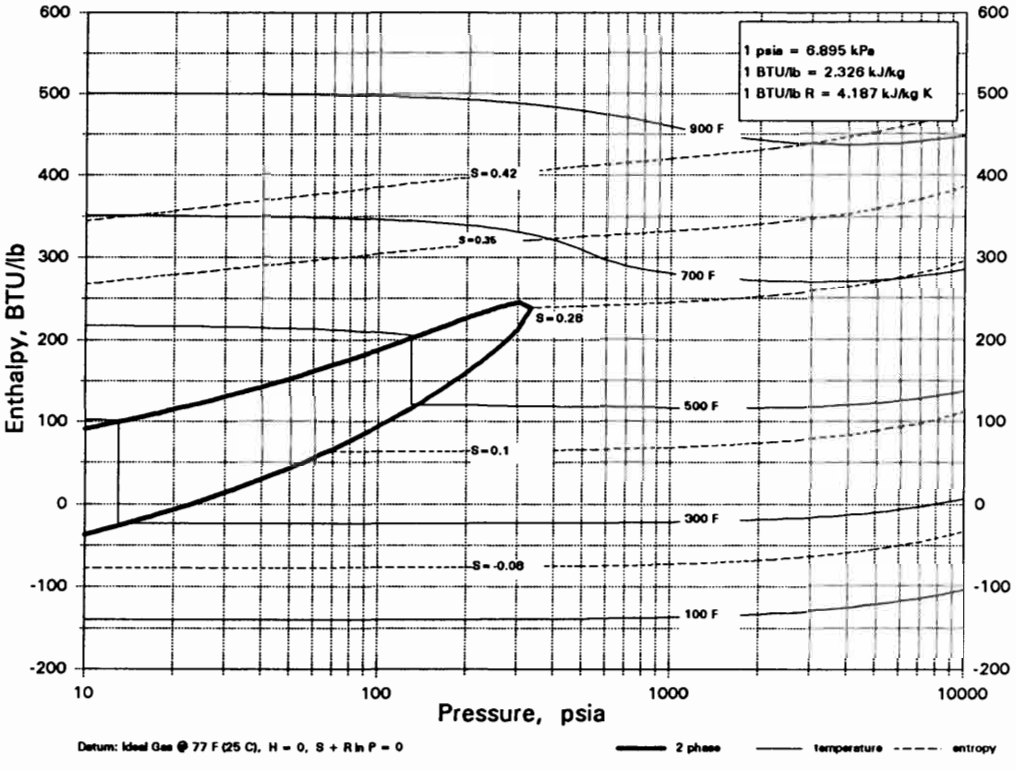
C9H20	4-METHYLOCTANE



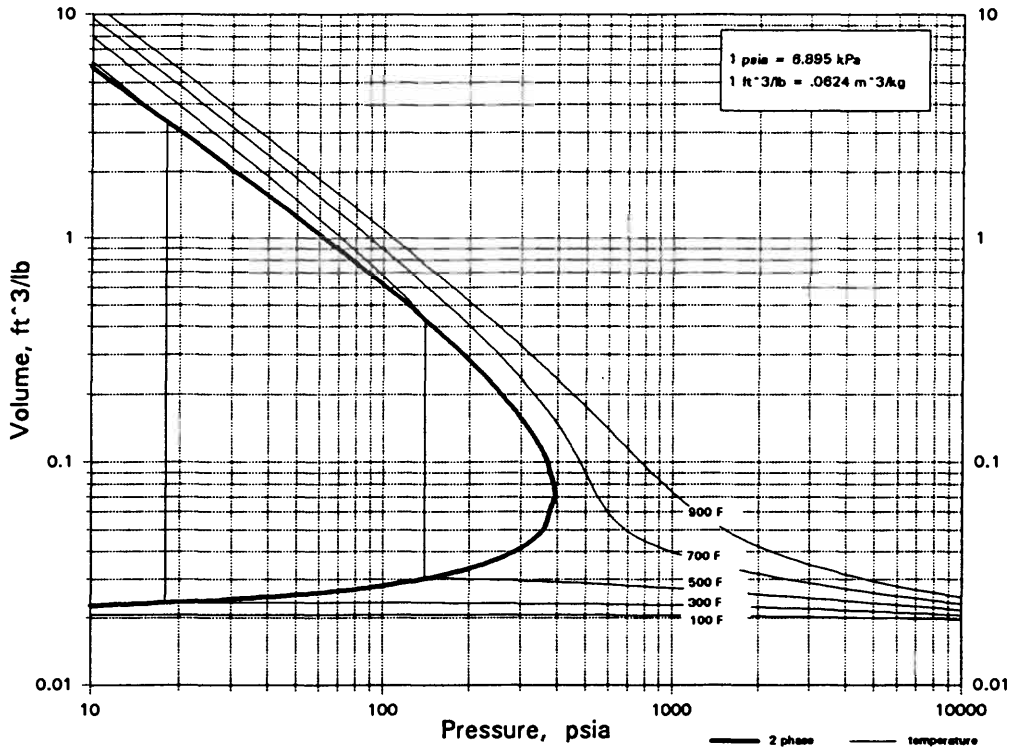


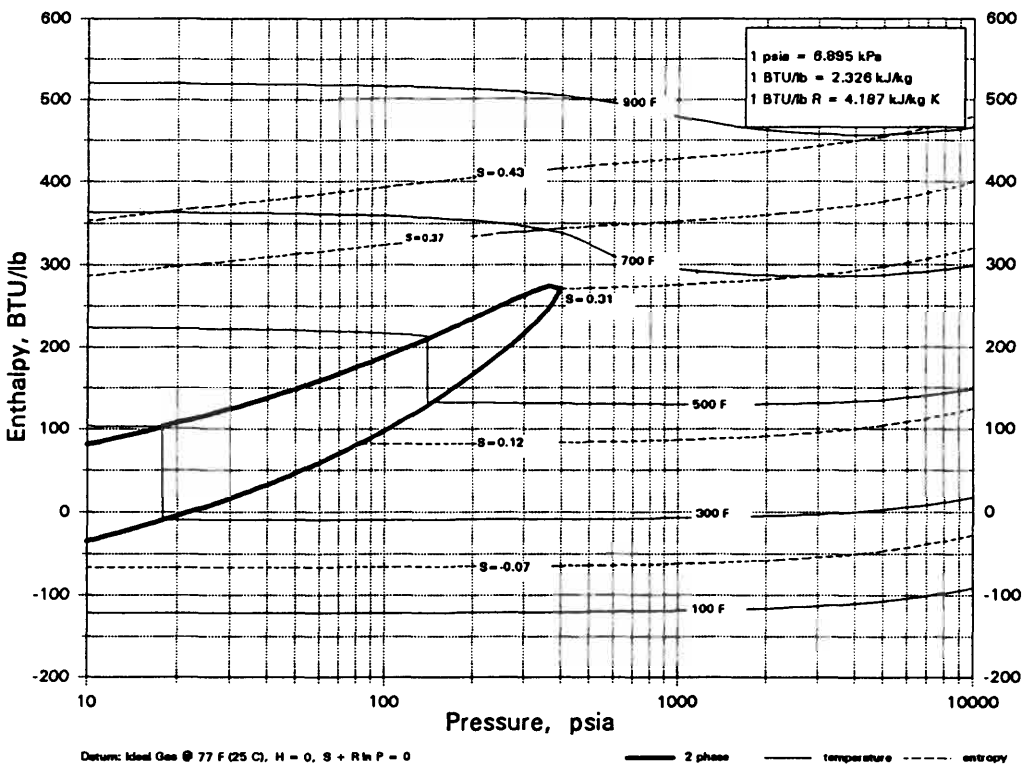
C9H20 n-NONANE



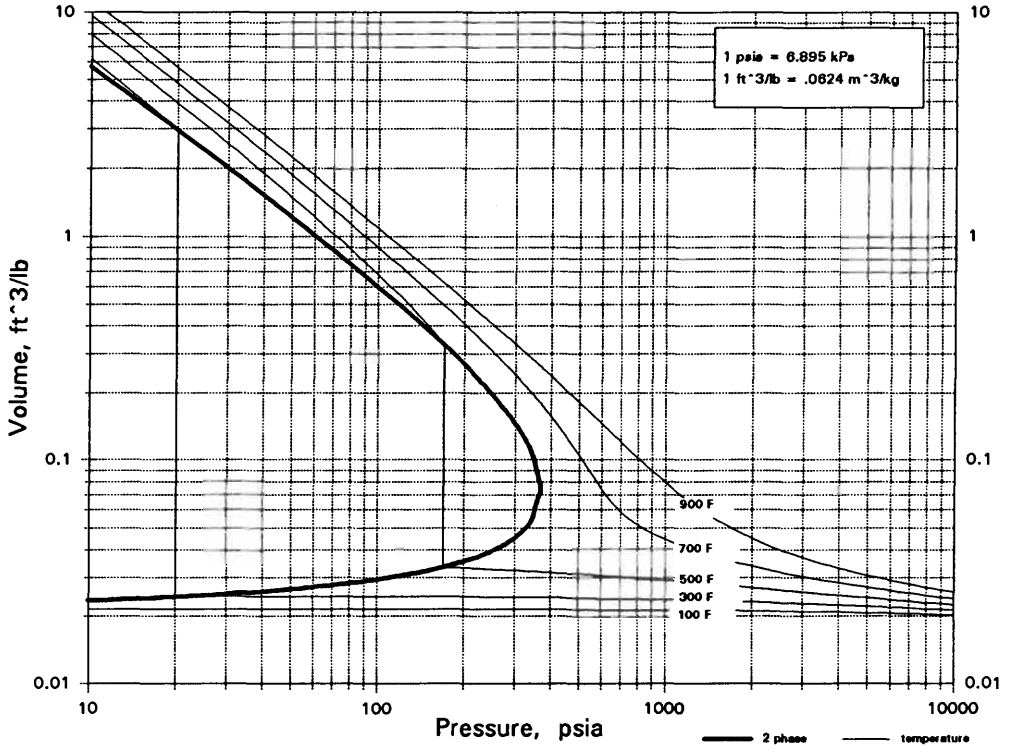


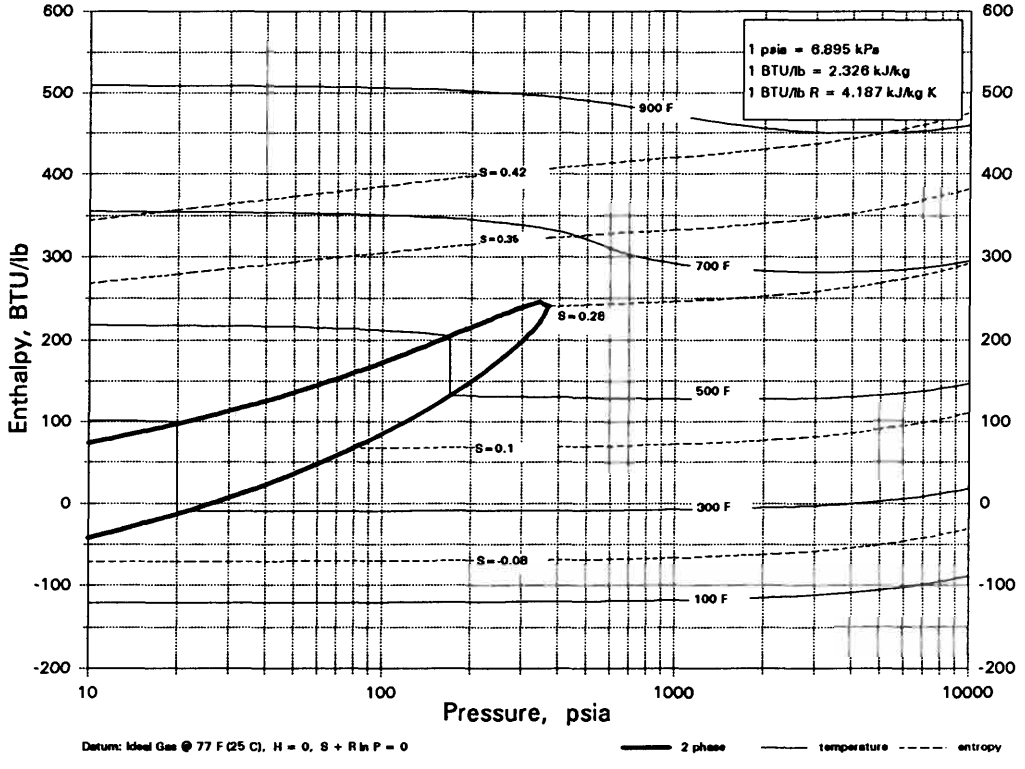
C9H20	2-2-3-3-TETRAMETHYLPENTANE



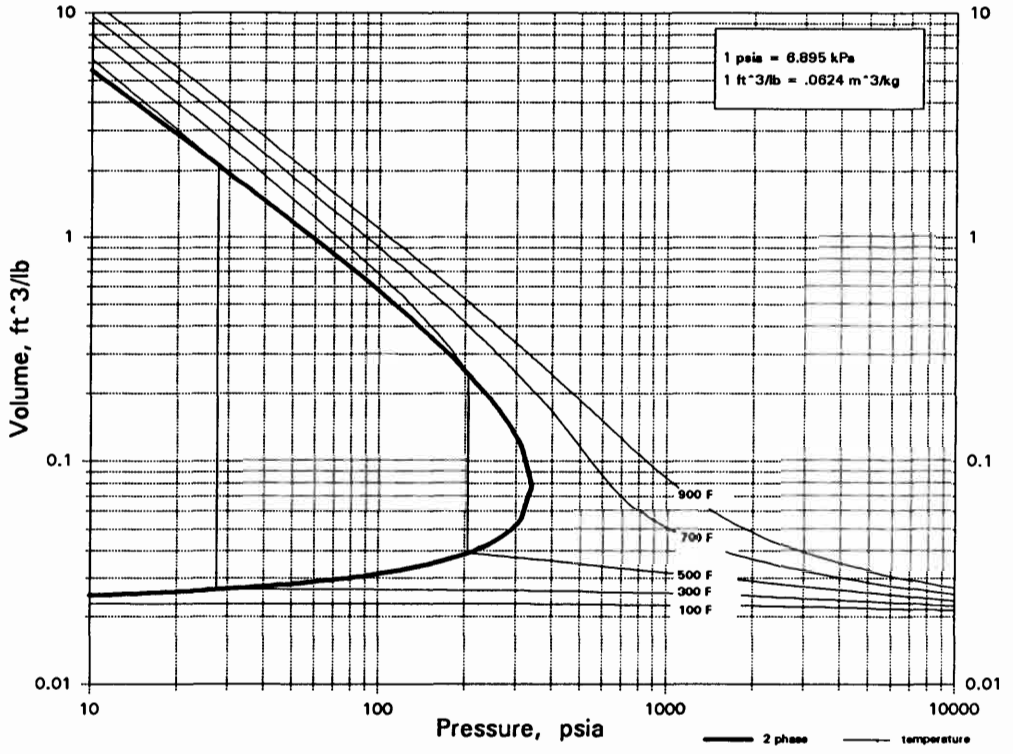


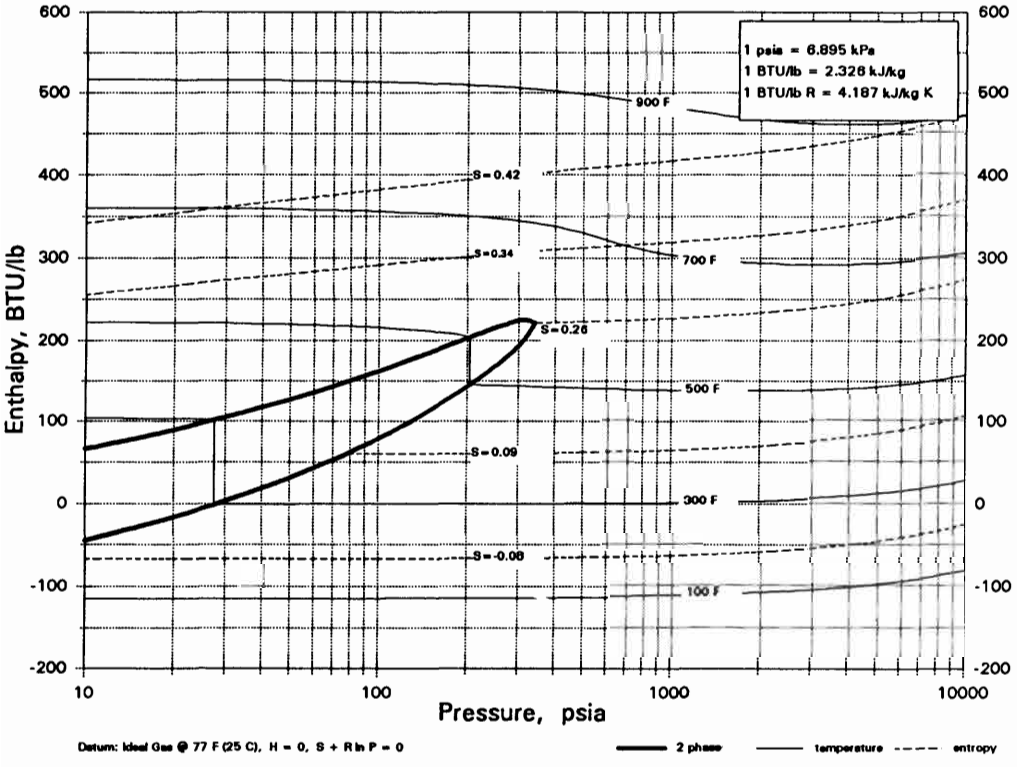
C9H20 2-2-3-4-TETRAMETHYLPENTANE



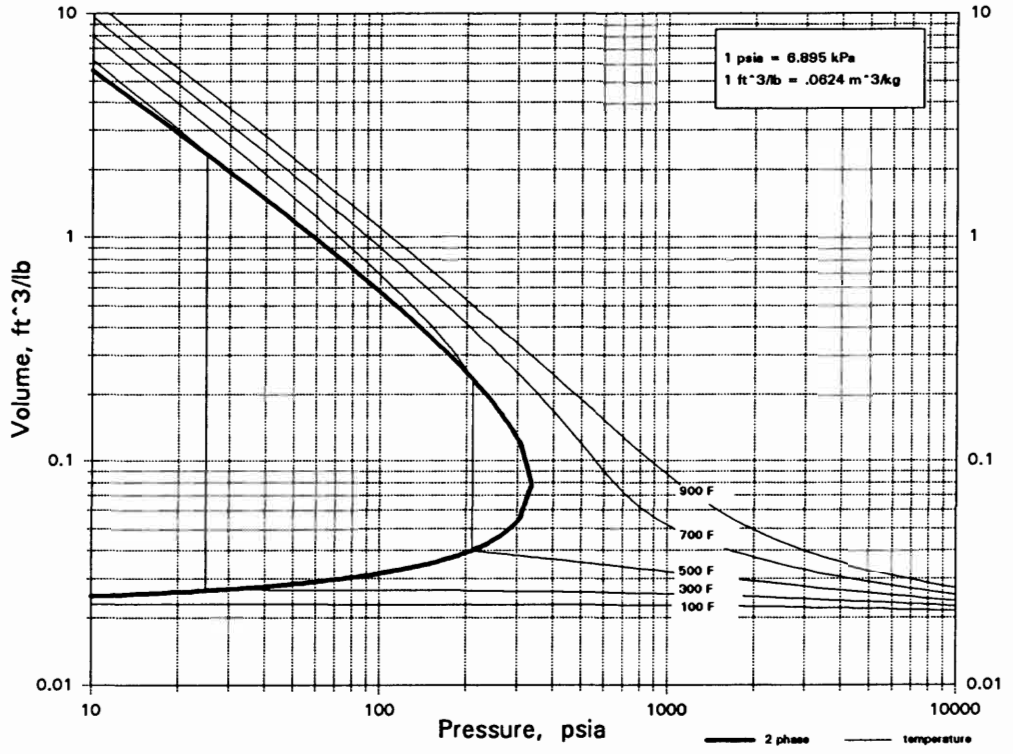


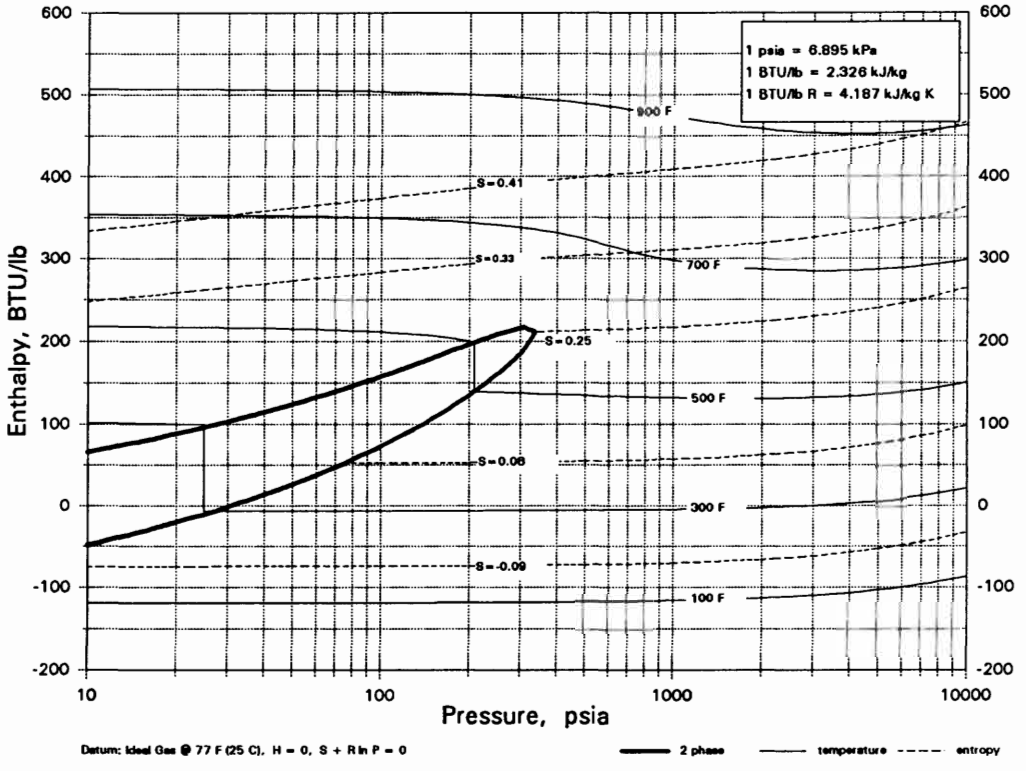
C9H20 2-2-4-4-TETRAMETHYLPENTANE



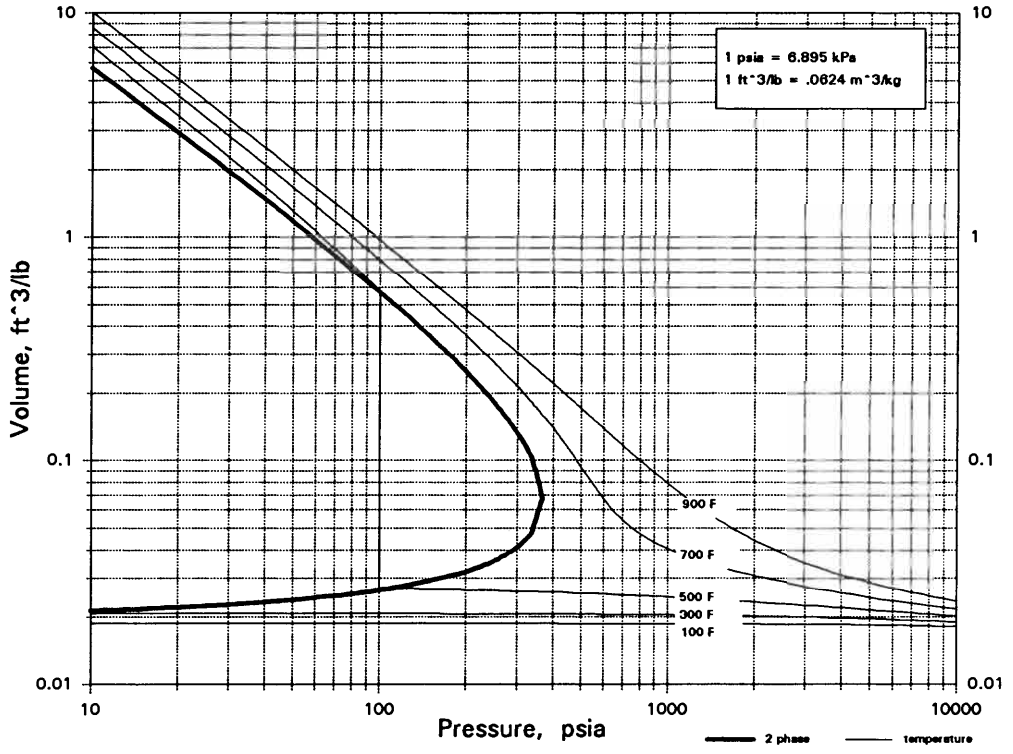


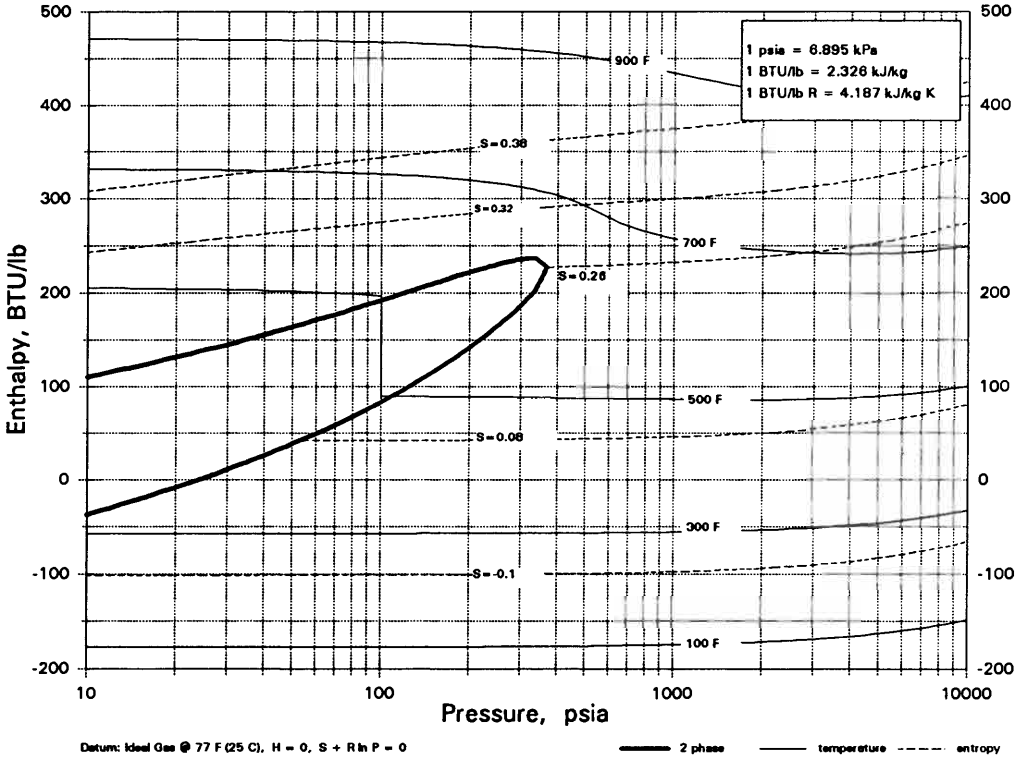
C9H20 2-2-5-TRIMETHYLHEXANE



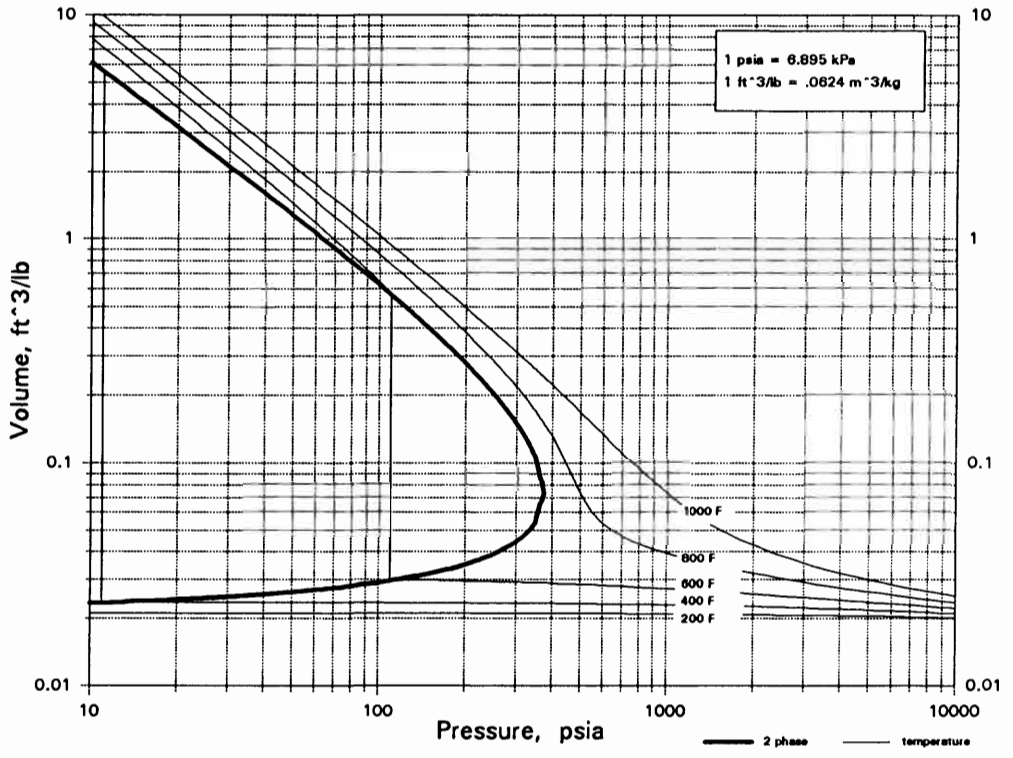


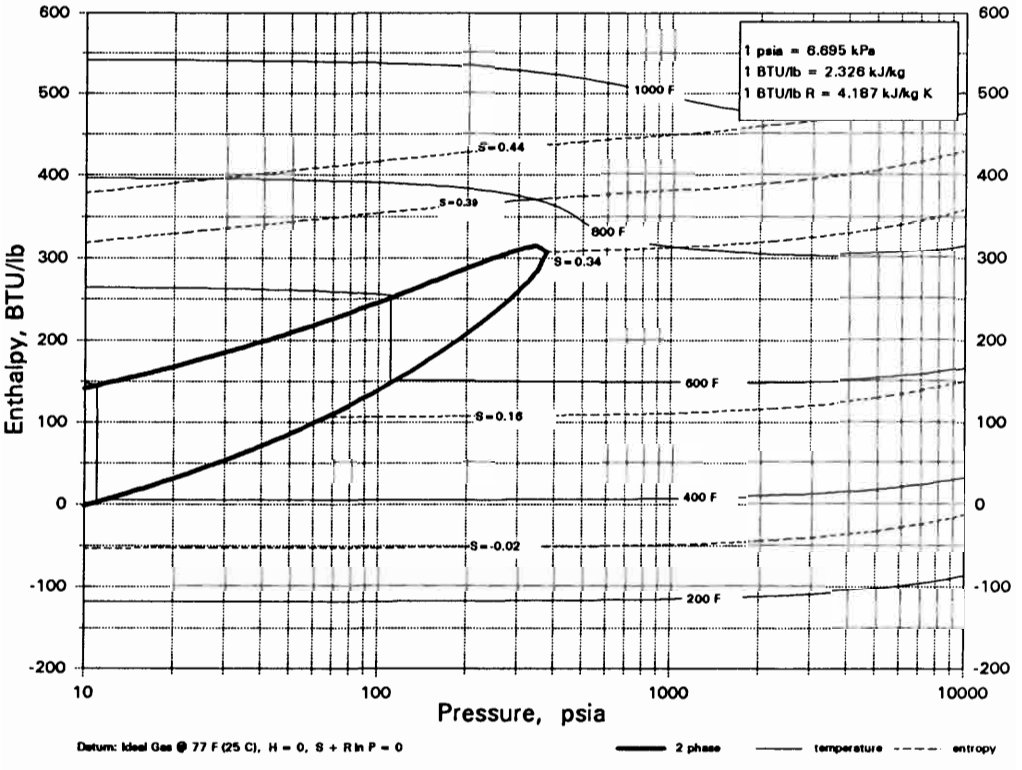
C9H20O	2-6-DIMETHYL-4-HEPTANOL



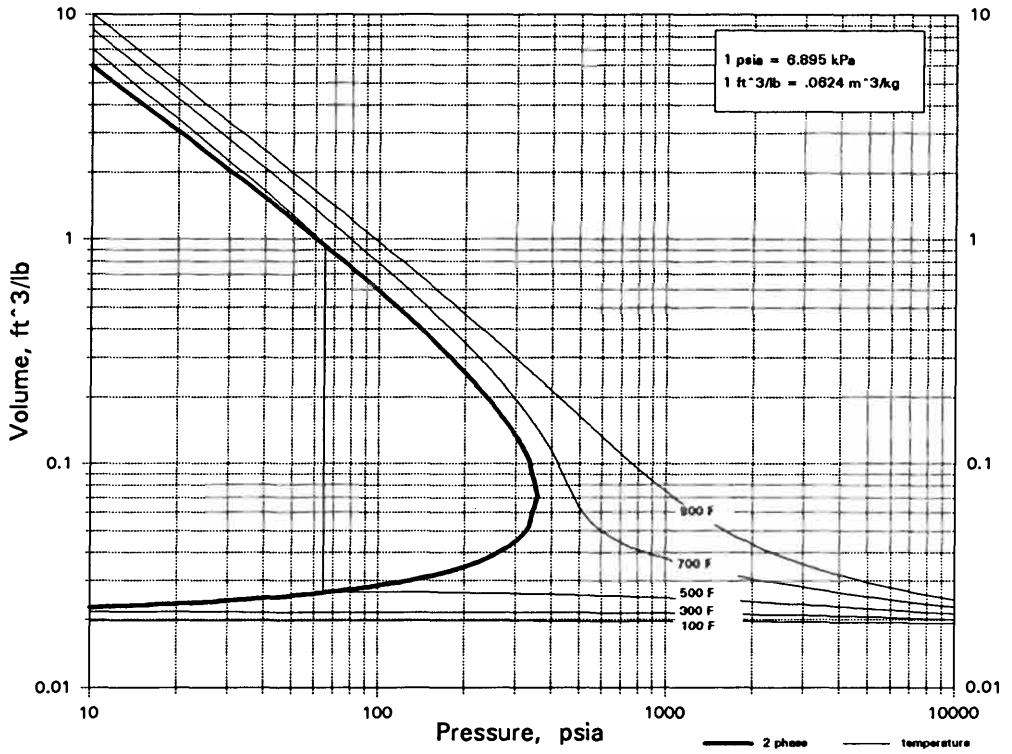


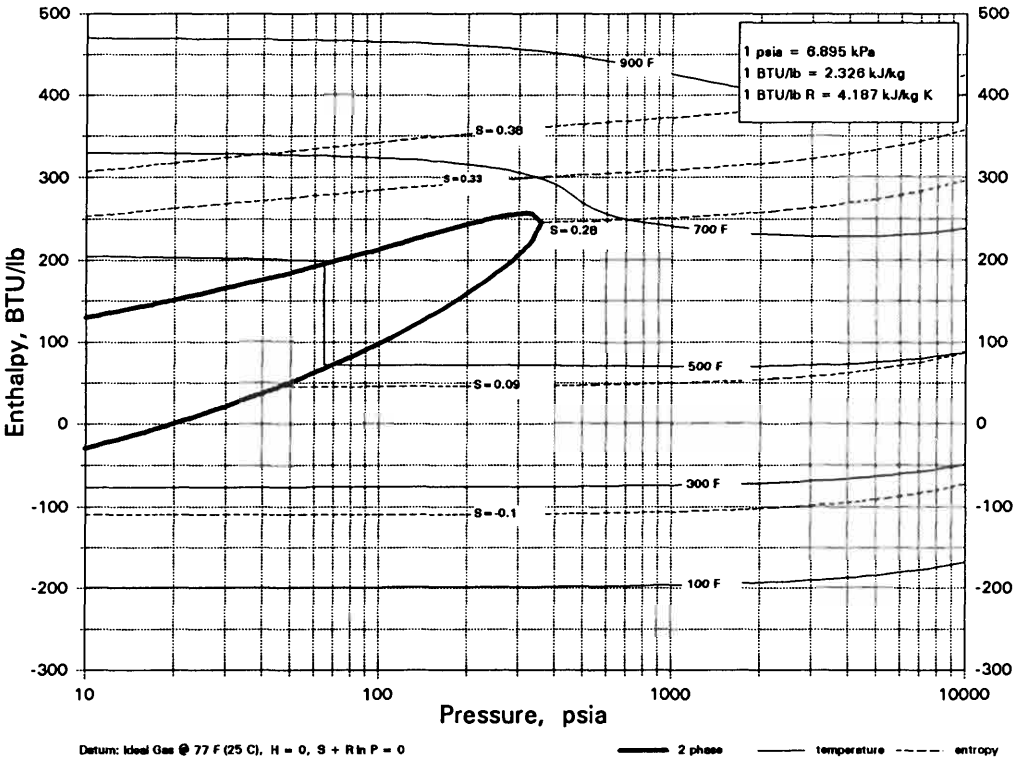
C9H20O 1-NONANOL



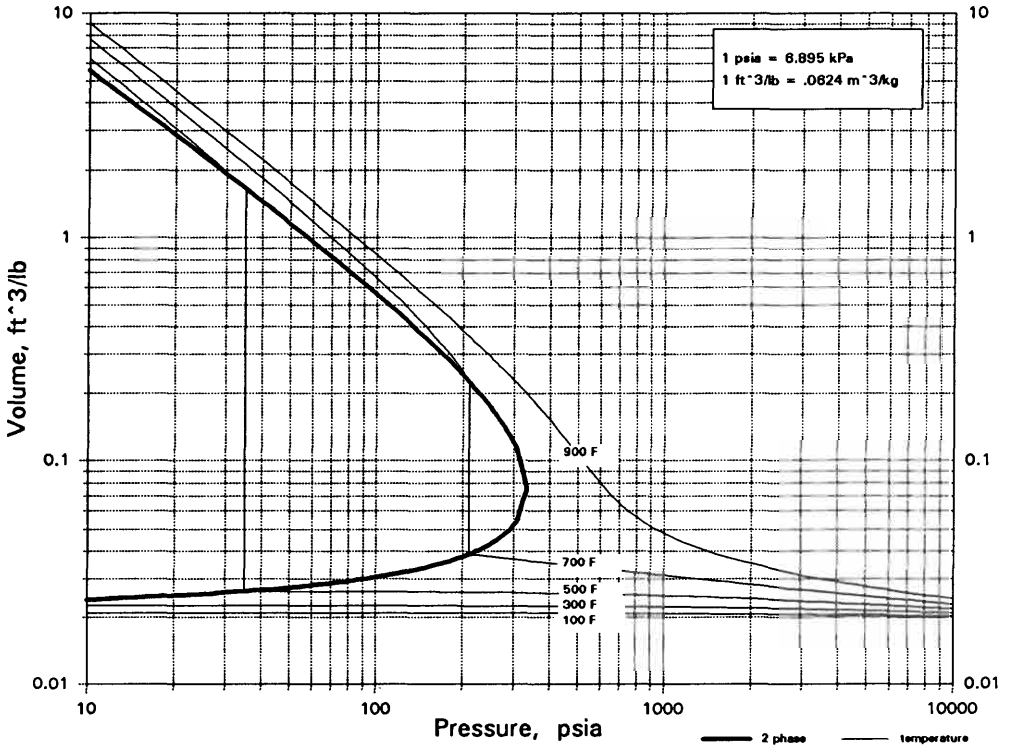


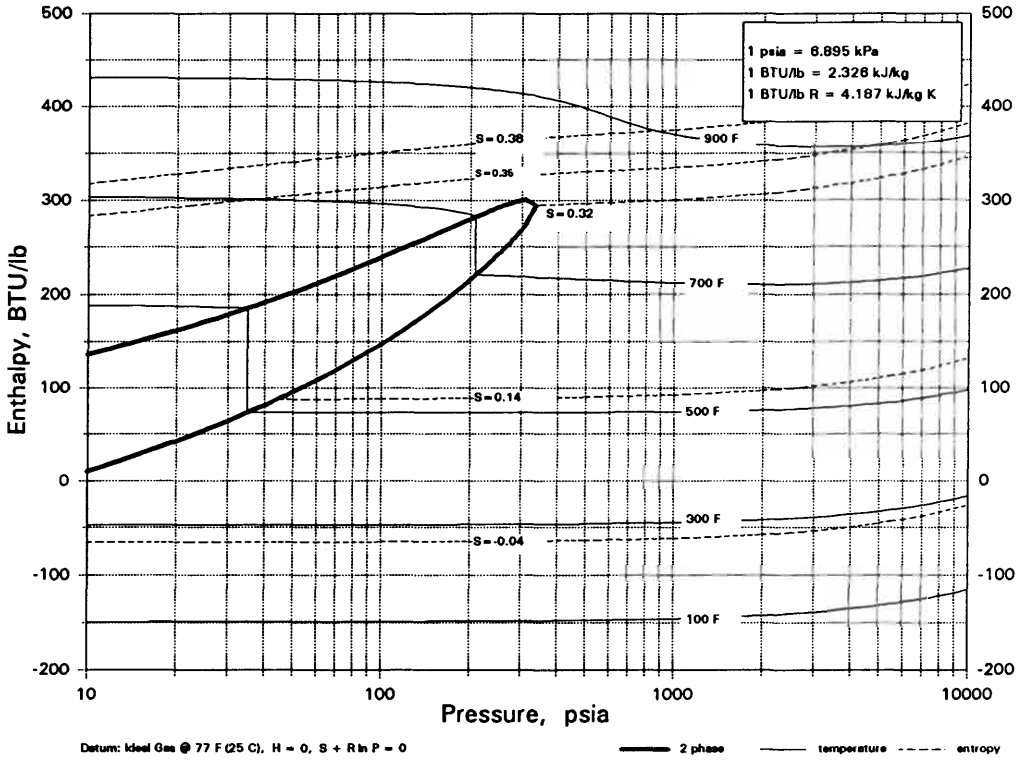
C9H20O 2-NONANOL



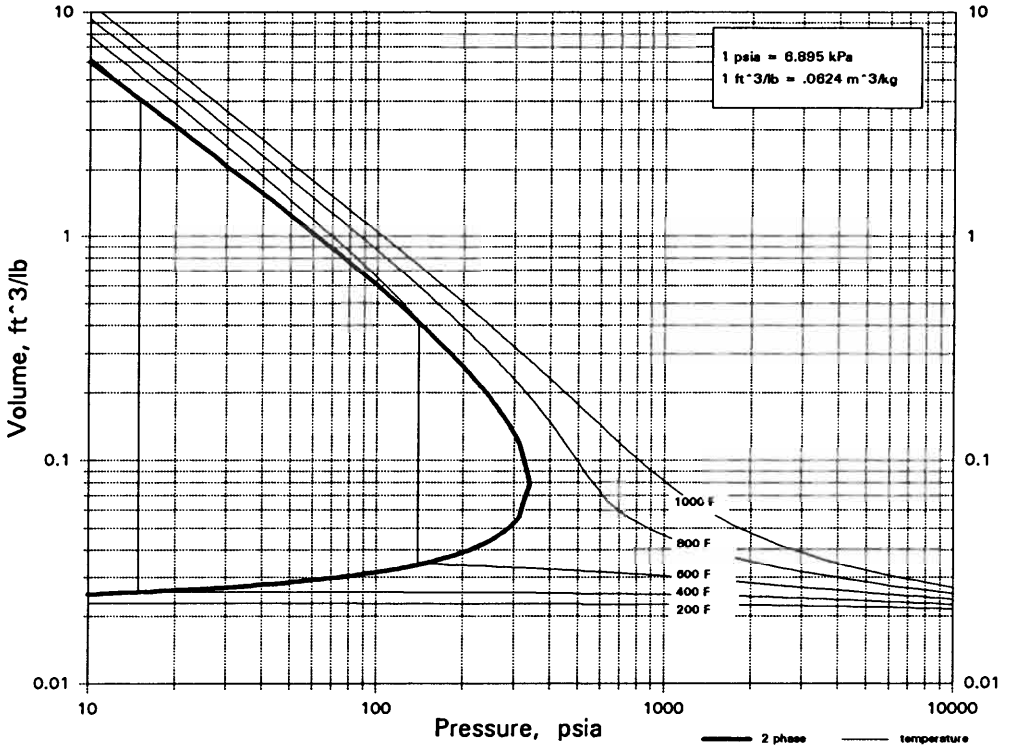


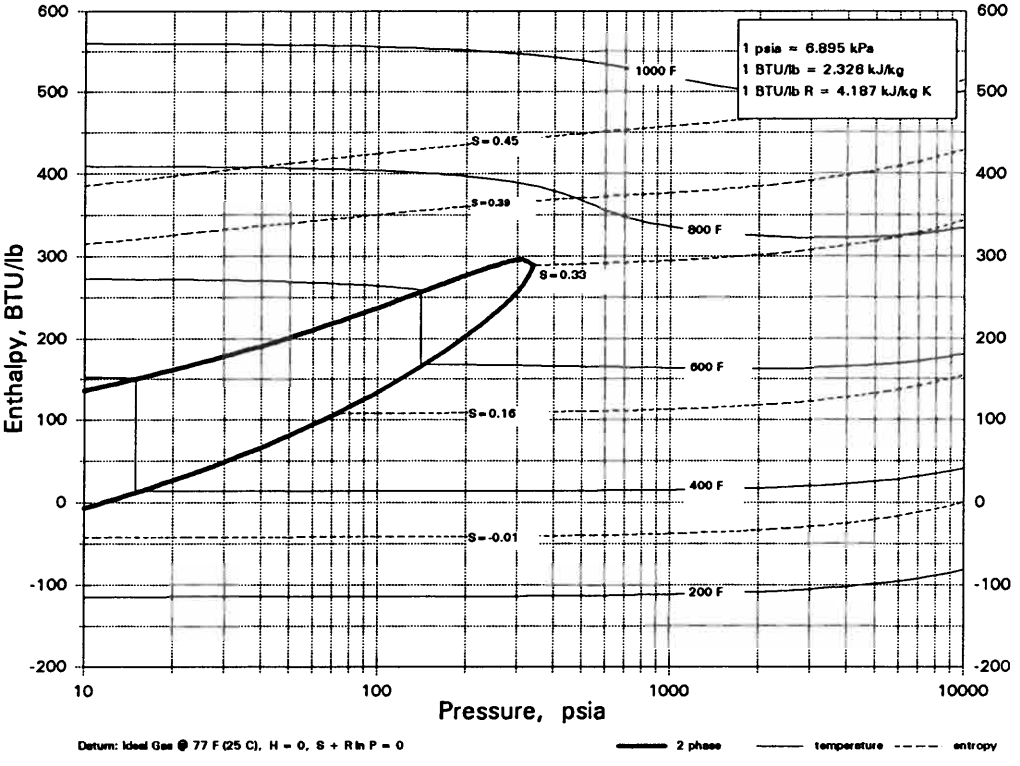
C9H20S n-NONYL MERCAPTAN



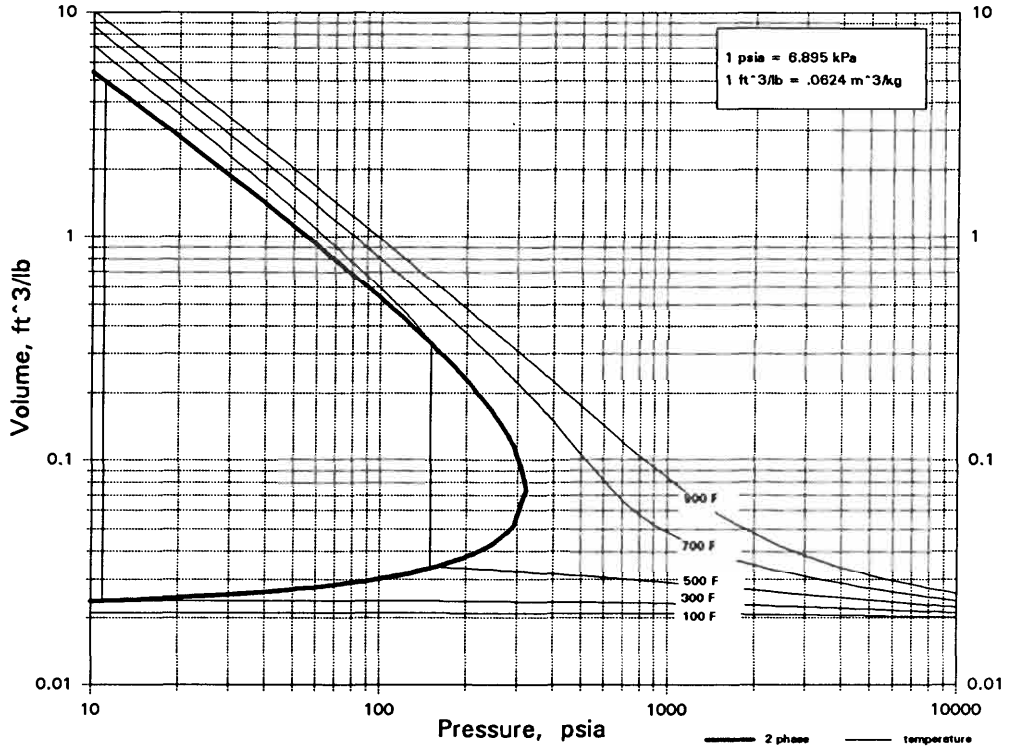


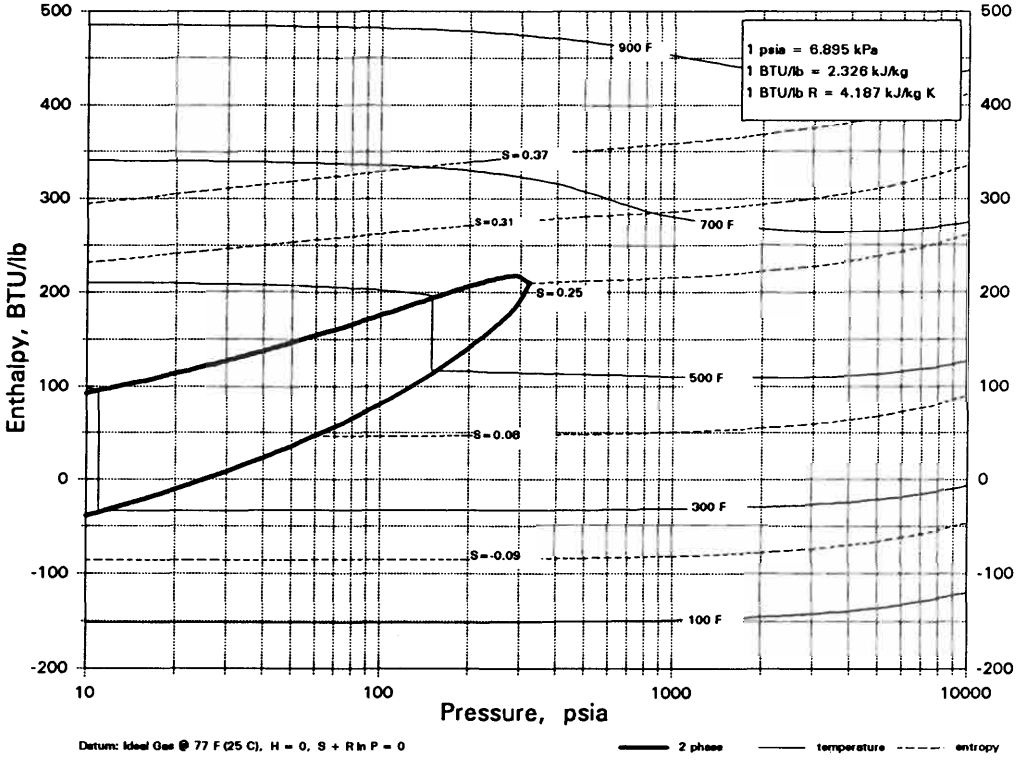
C9H21N n-NONYLAMINE



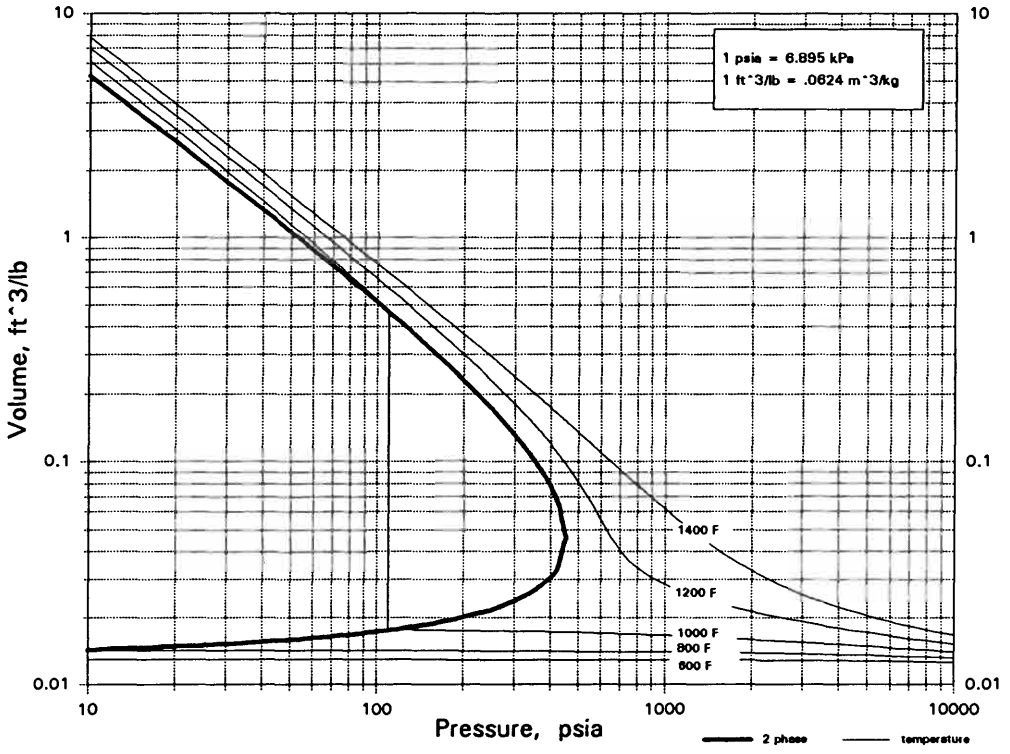


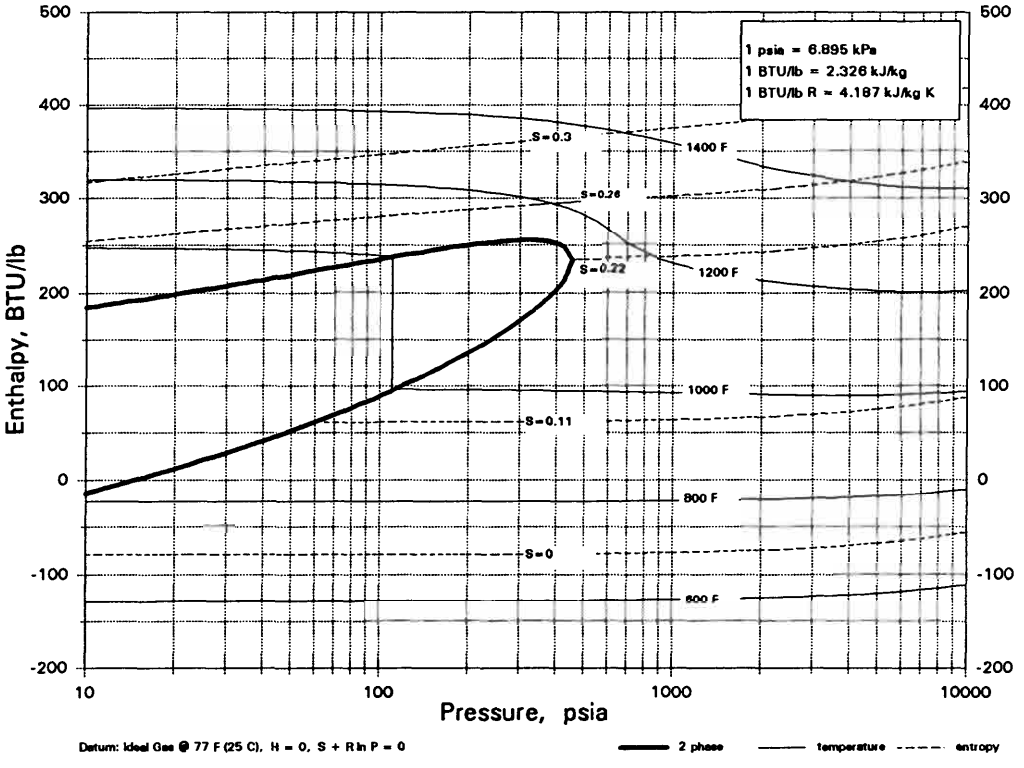
C9H21N TRIPROPYLAMINE



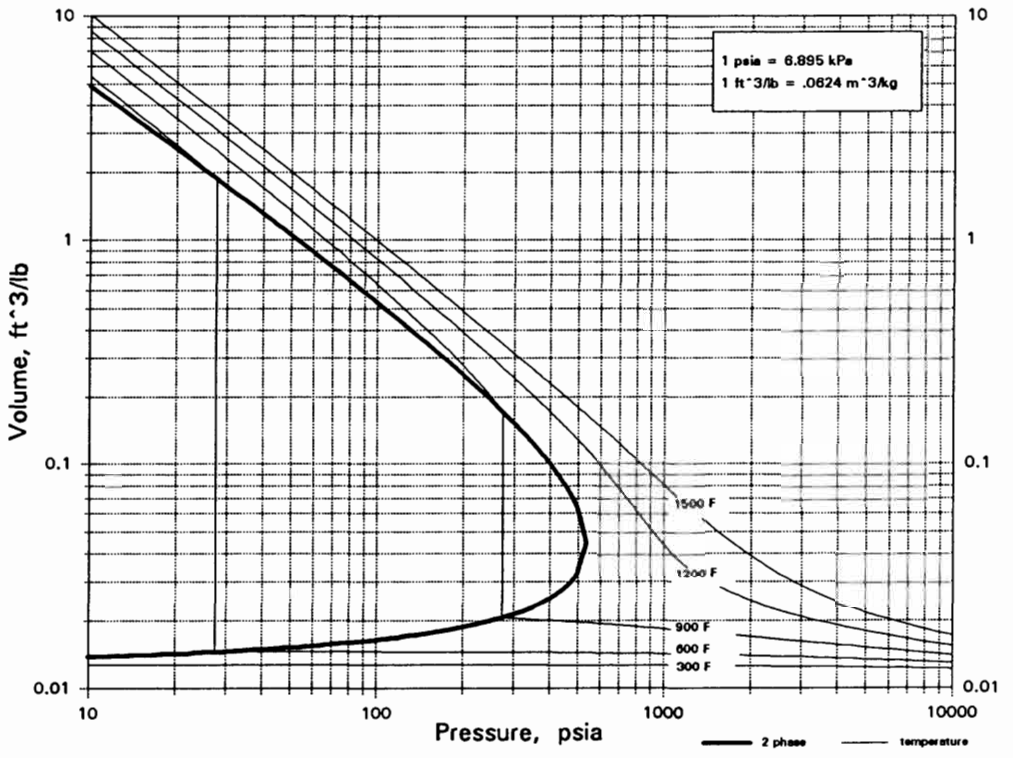


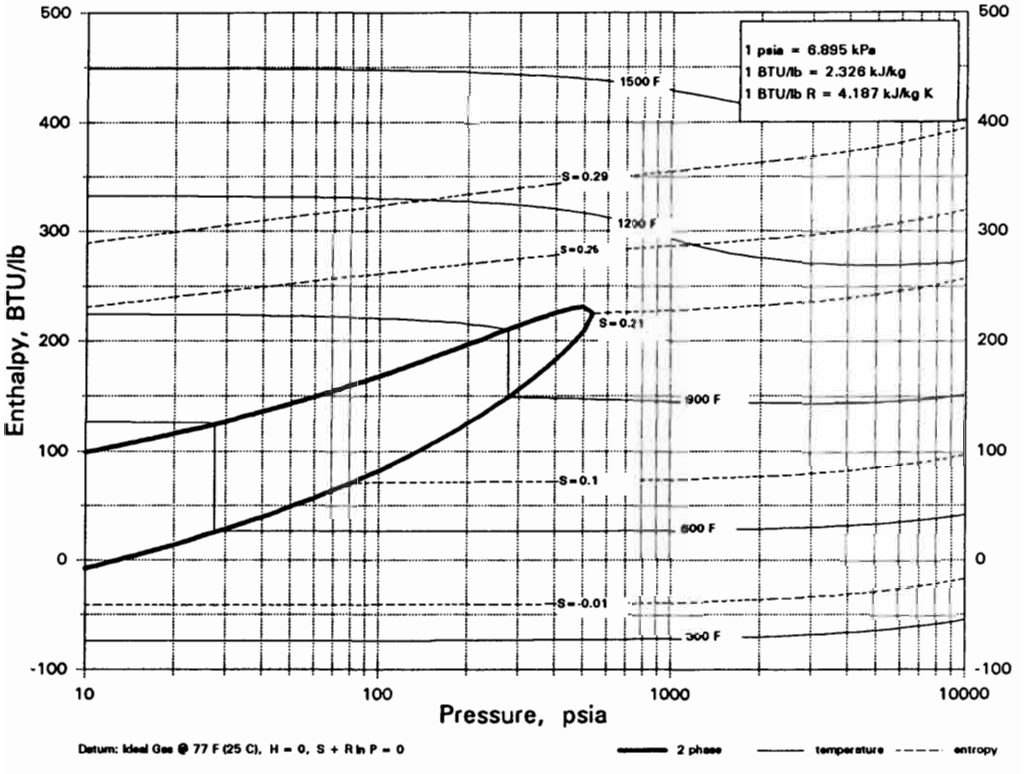
C10H6O8 PYROMELLITIC ACID



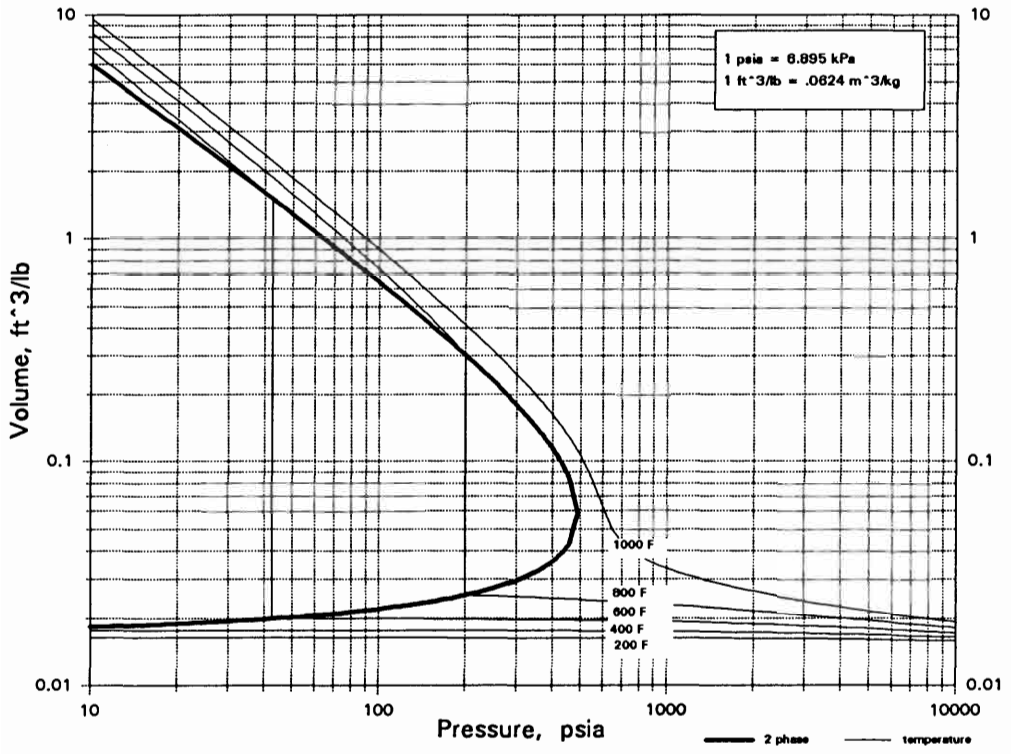


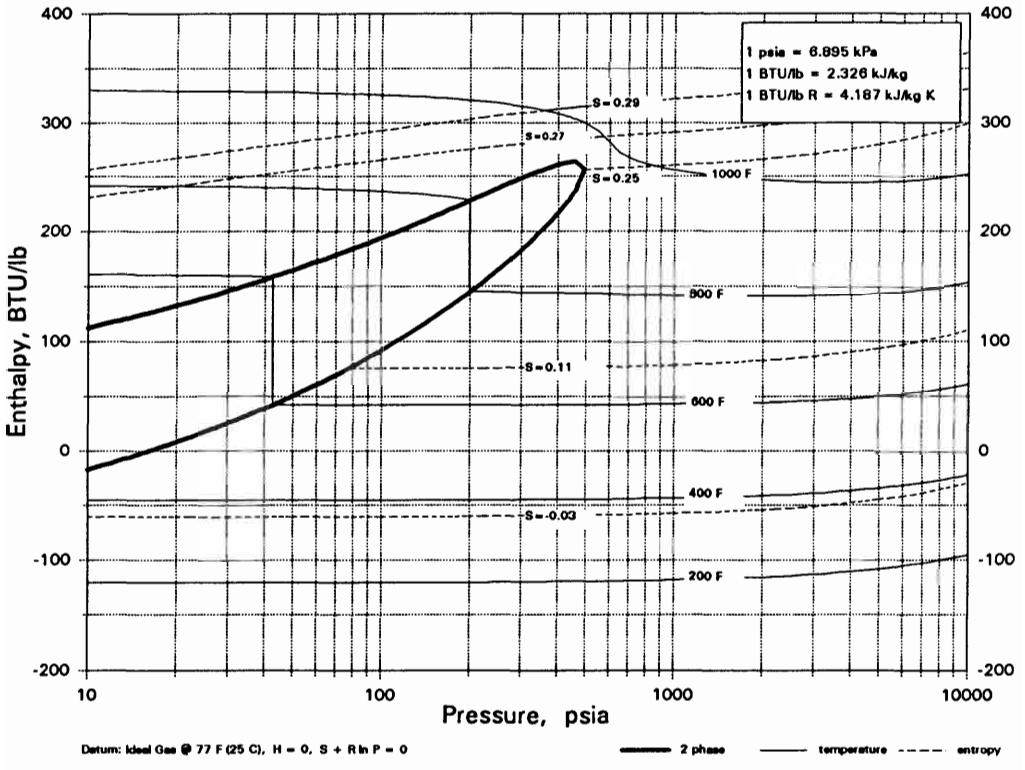
C10H7Br 1-BROMONAPHTHALENE



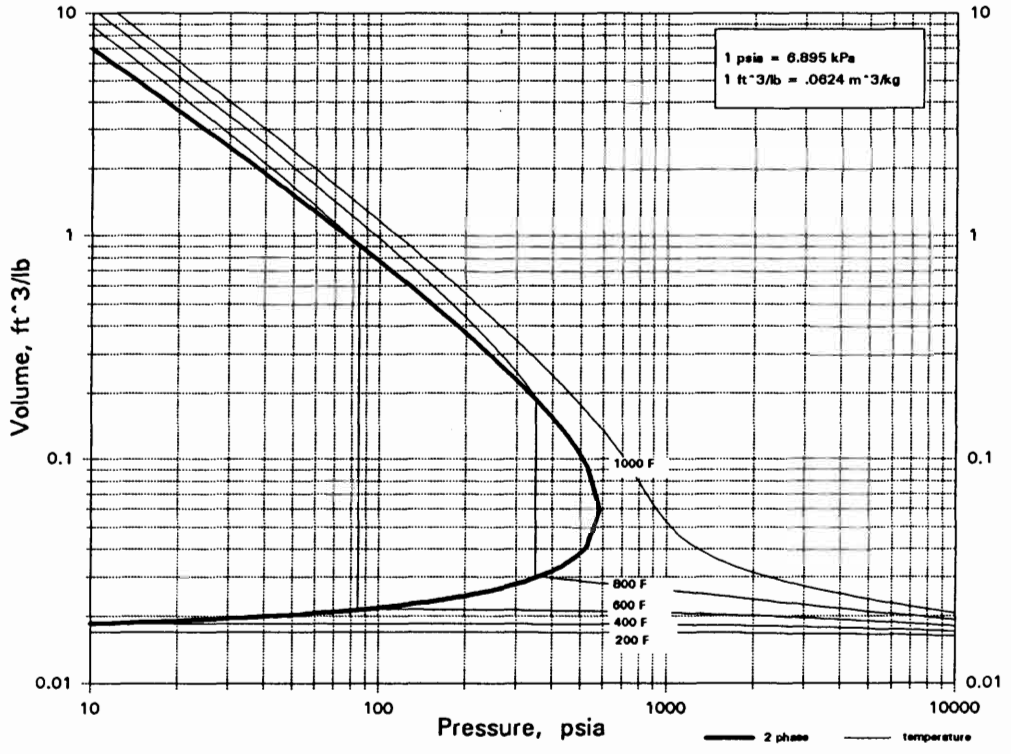


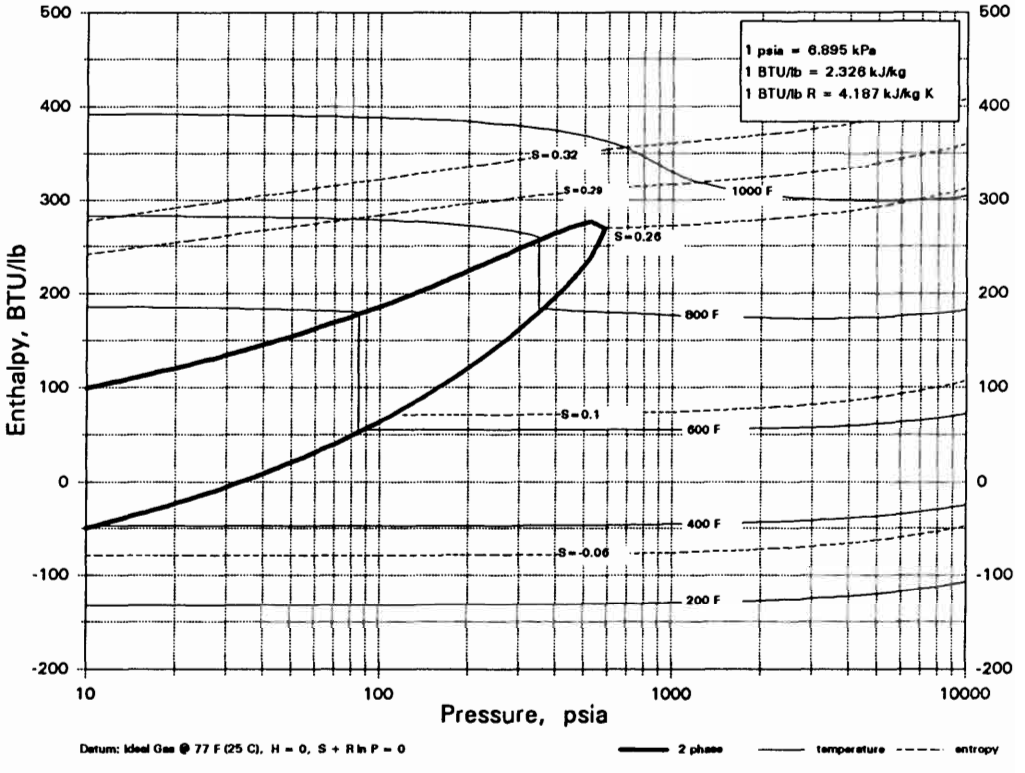
C10H7Cl 1-CHLORONAPHTHALENE



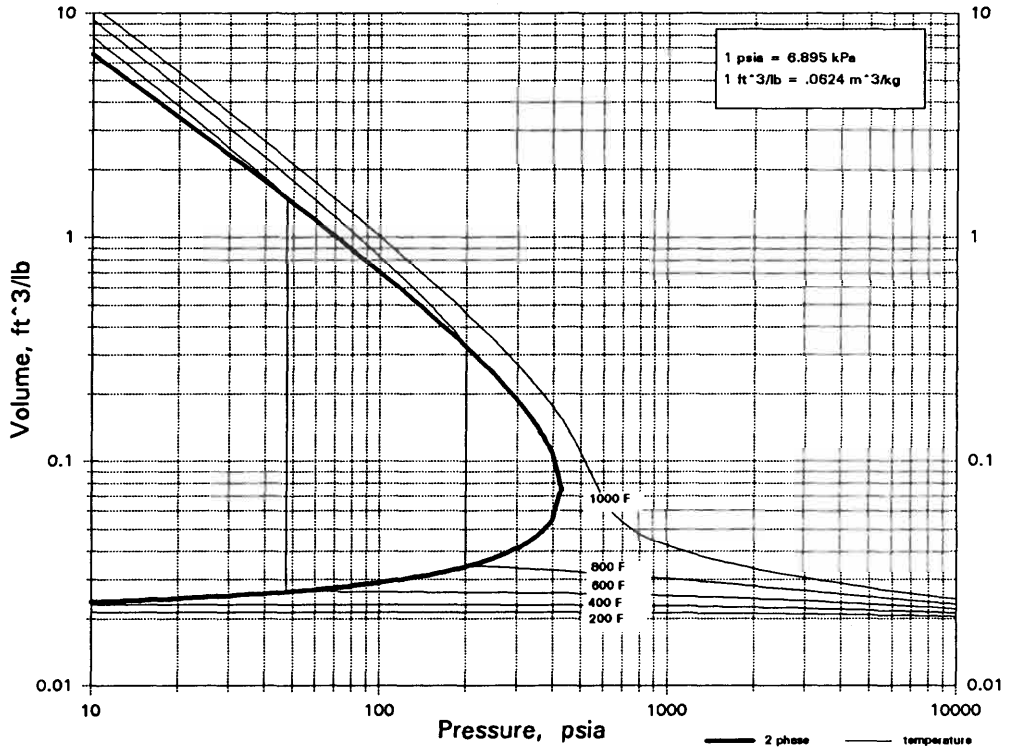


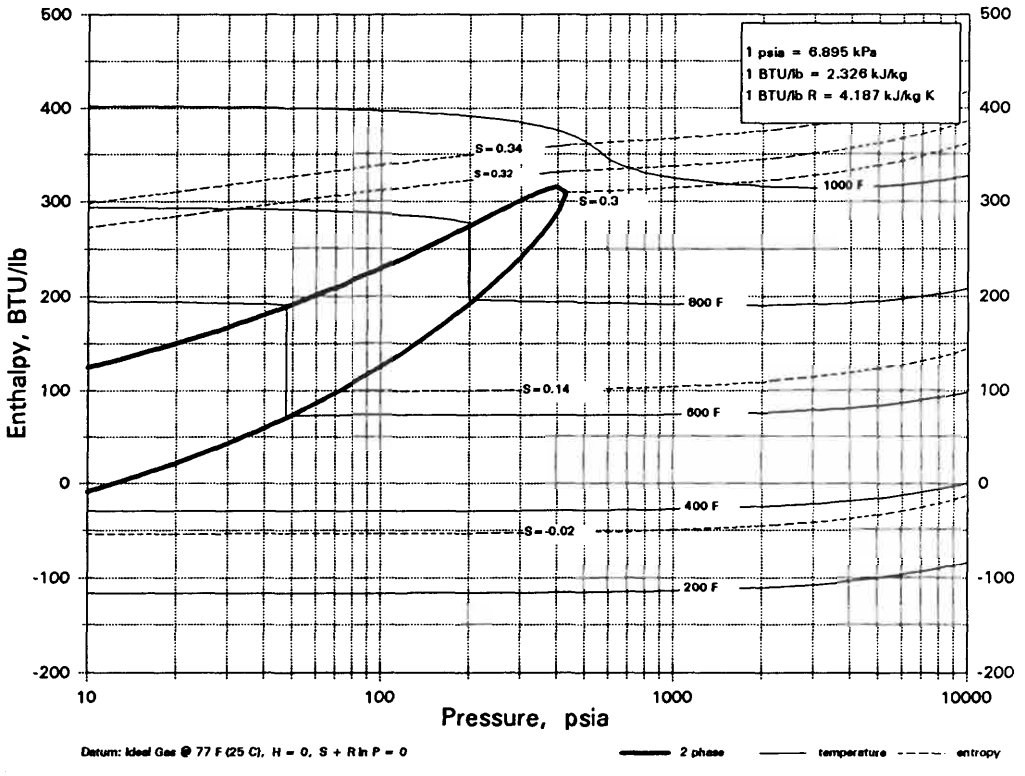
C10H8 NAPHTHALENE



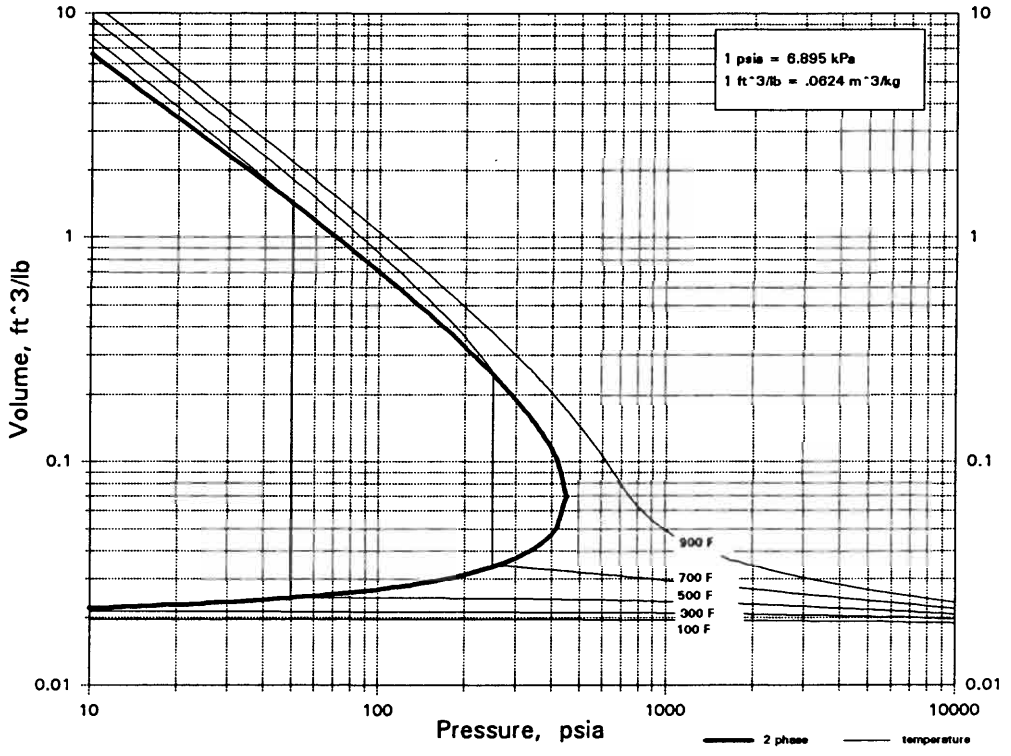


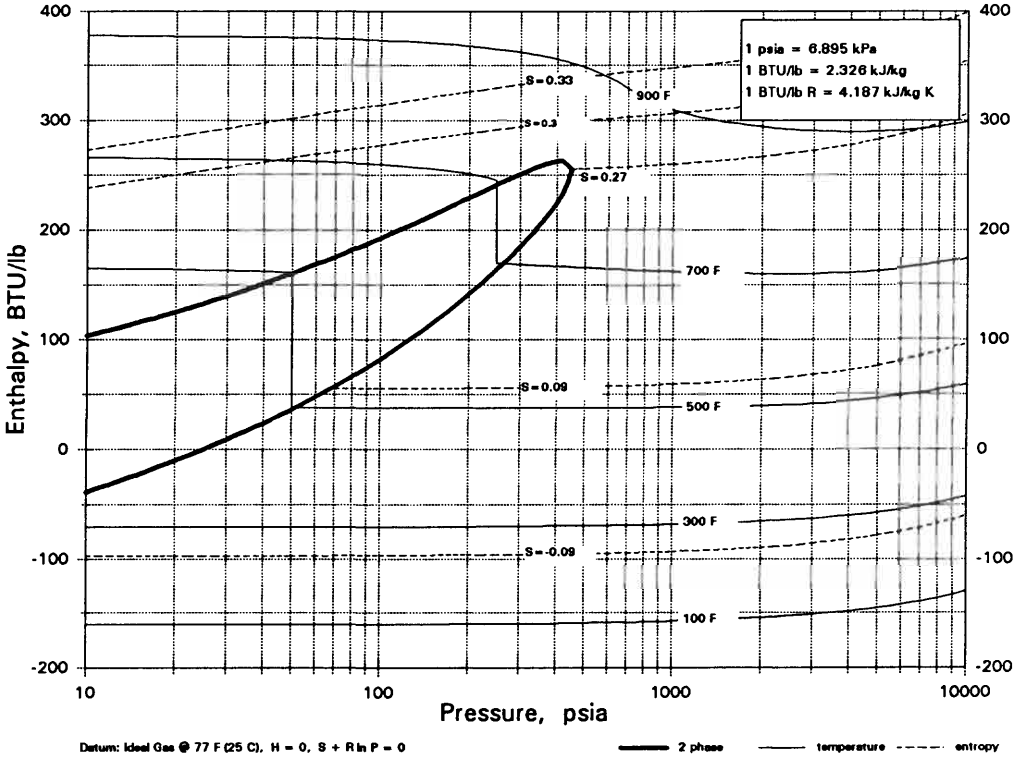
C10H9N QUINALDINE



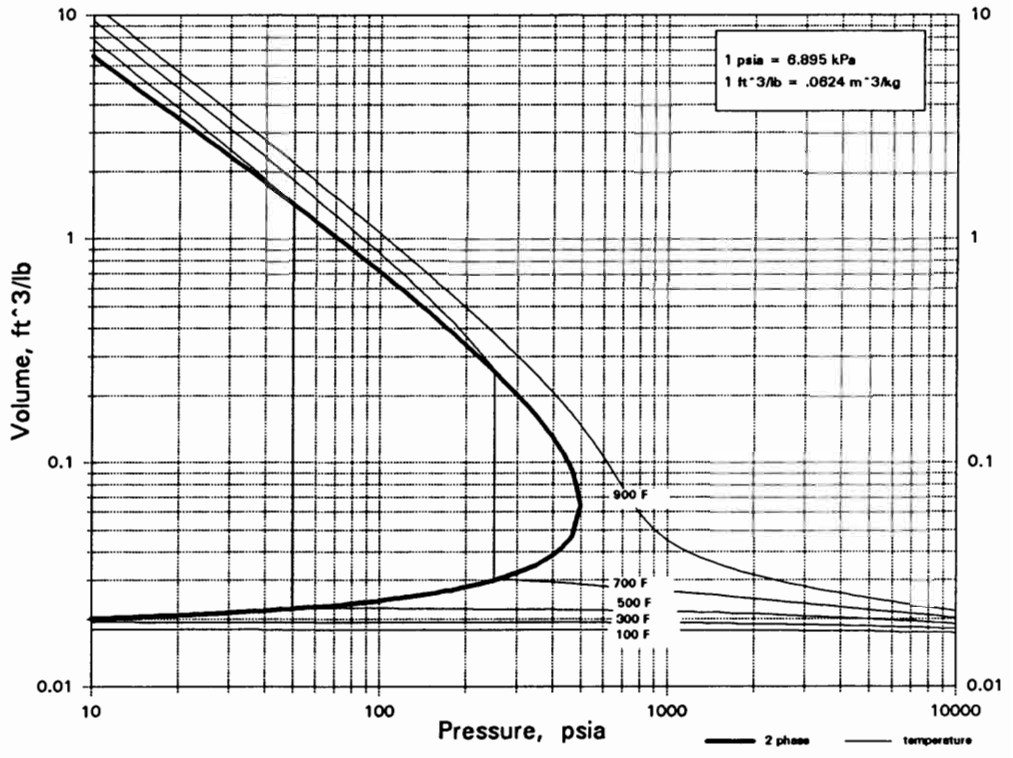


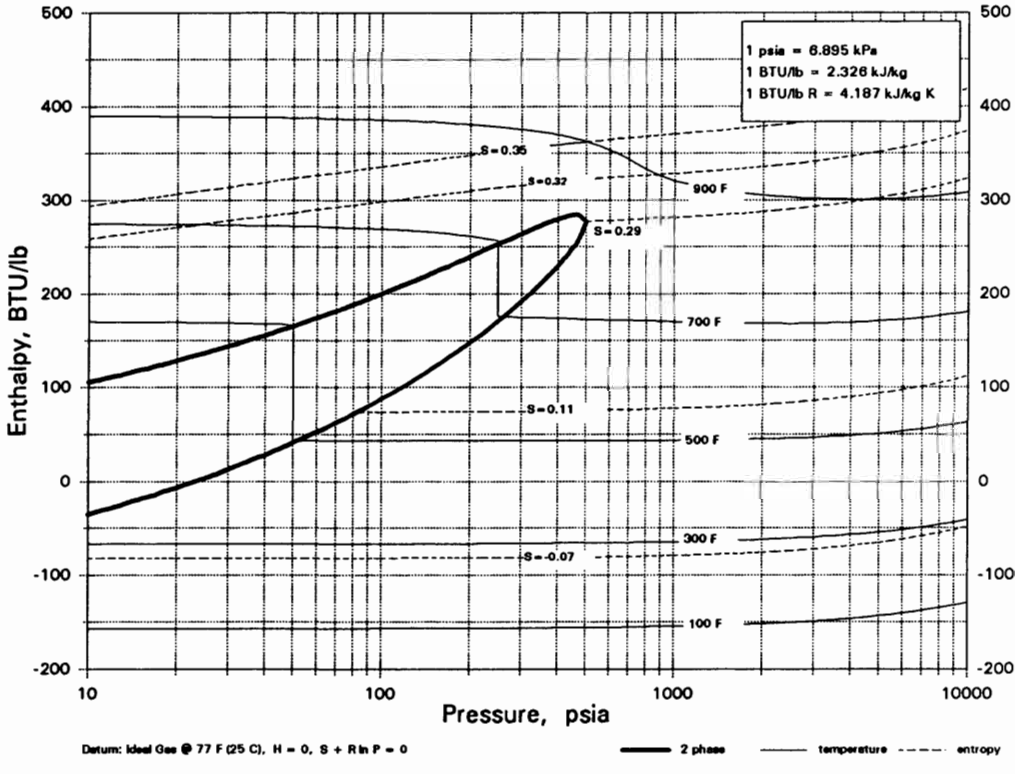
C10H10 m-DIVINYLBENZENE



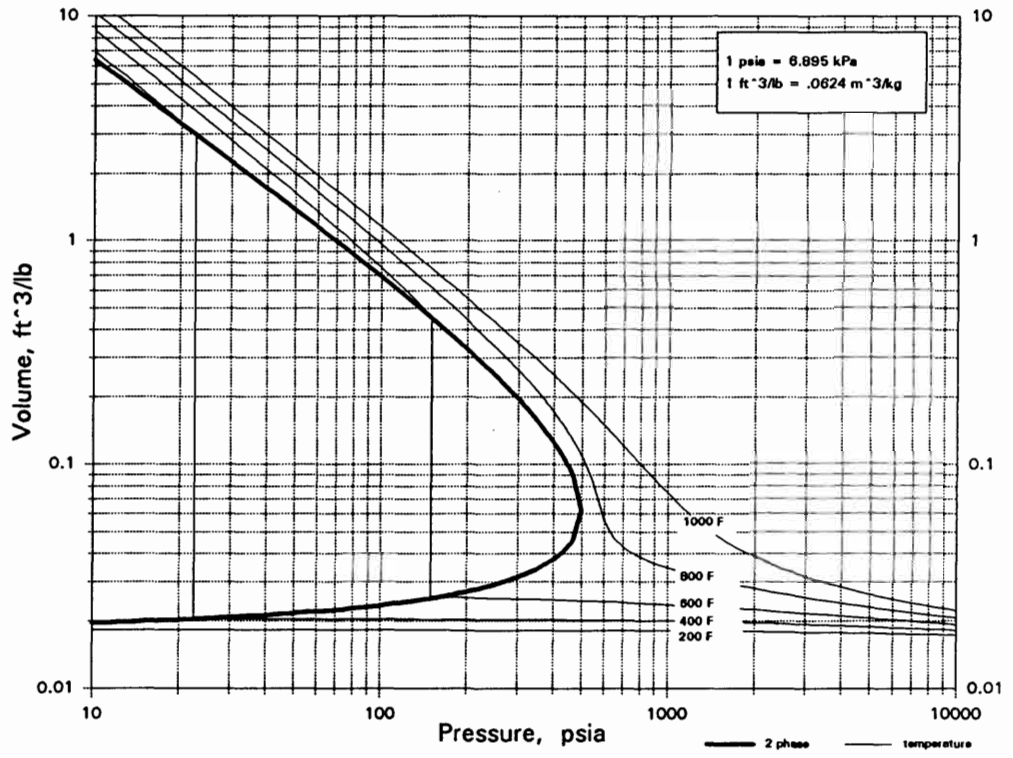


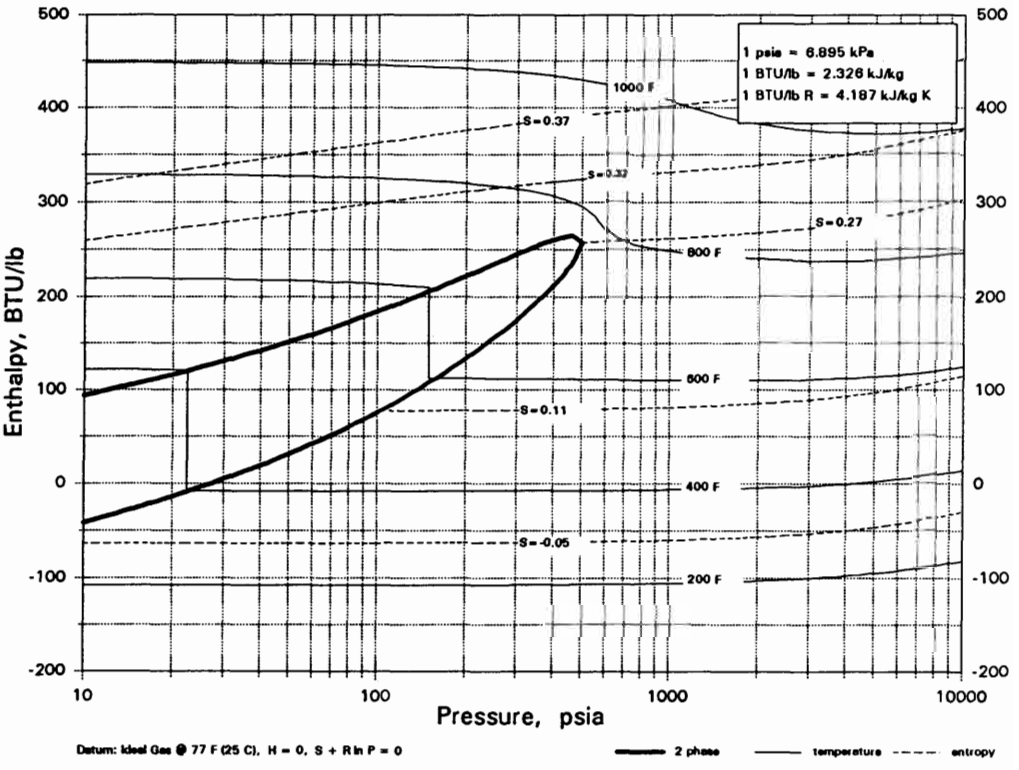
C10H10 1-METHYLINDENE



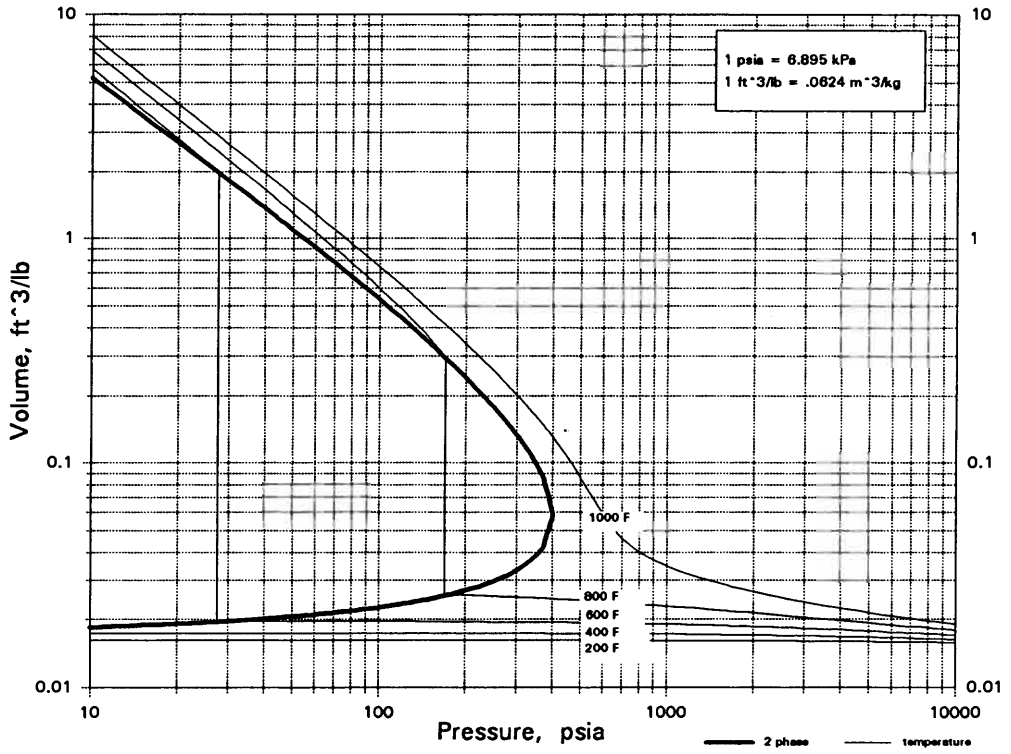


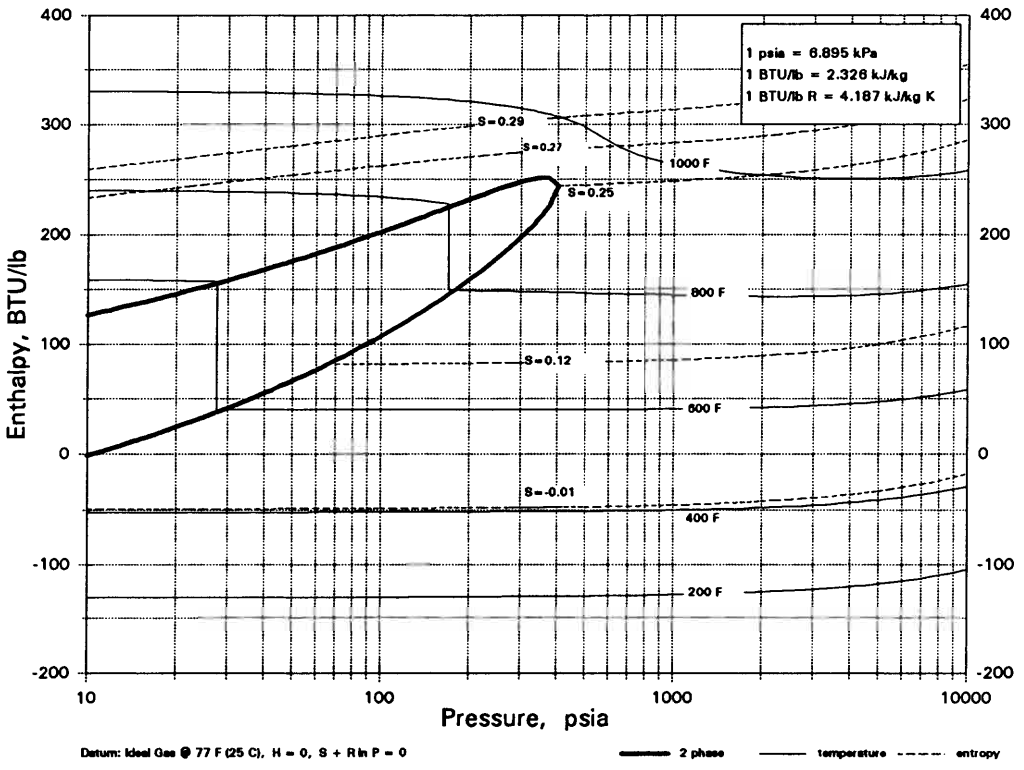
C10H10 2-METHYLINDENE



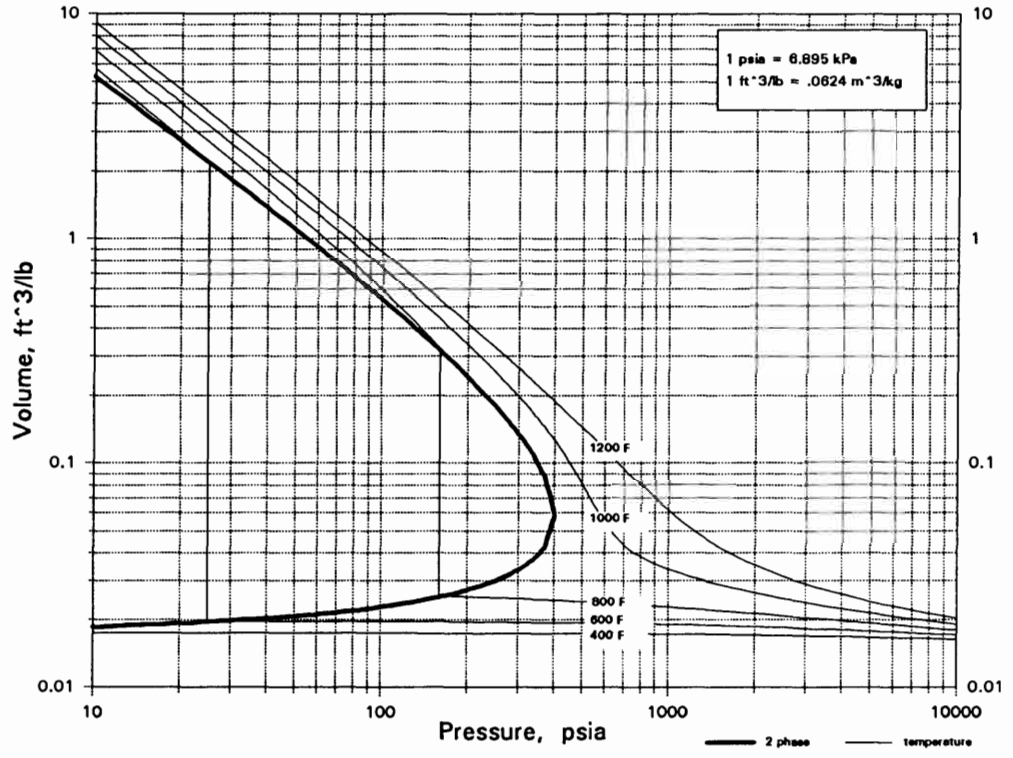


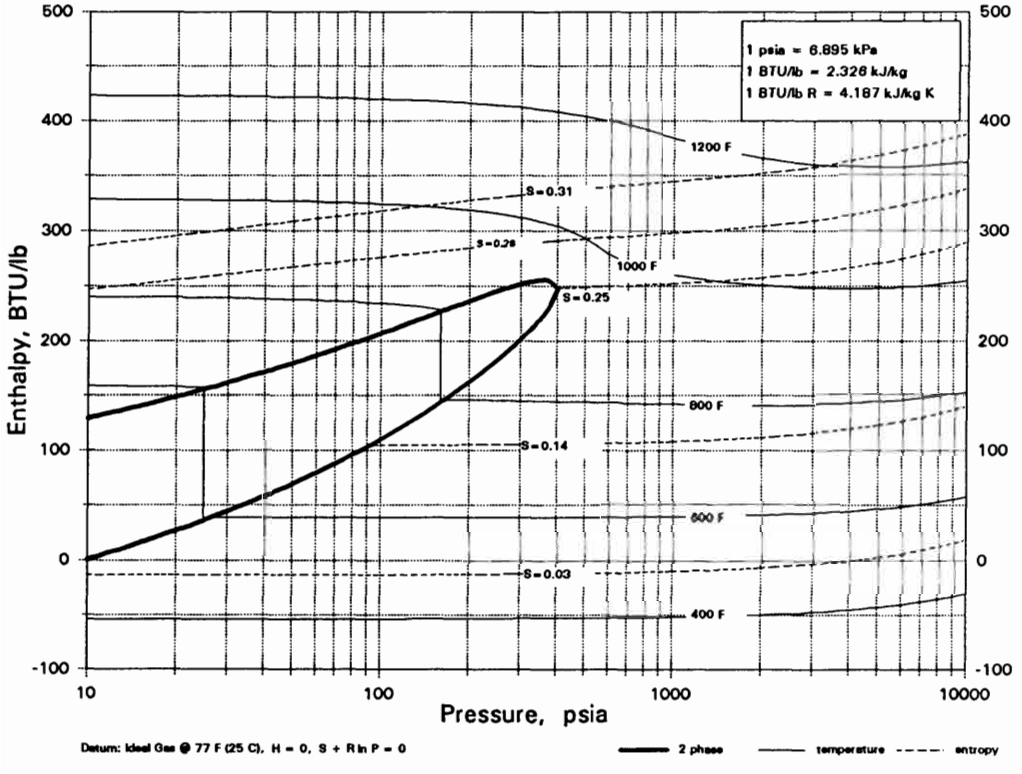
C10H10O4 DIMETHYL PHTHALATE



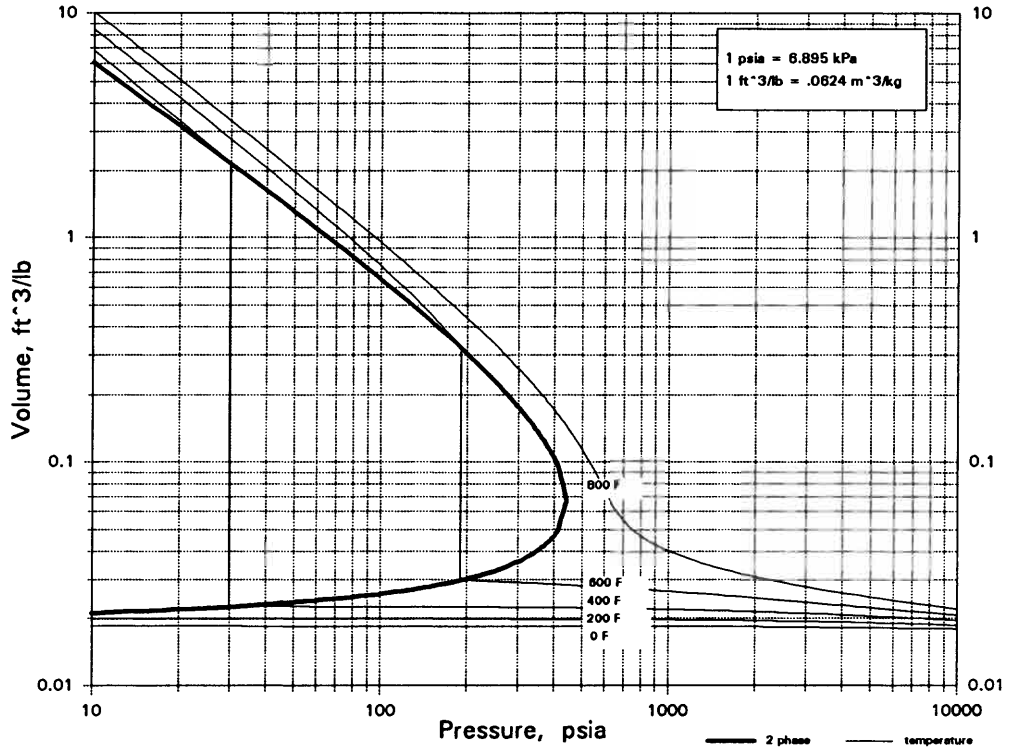


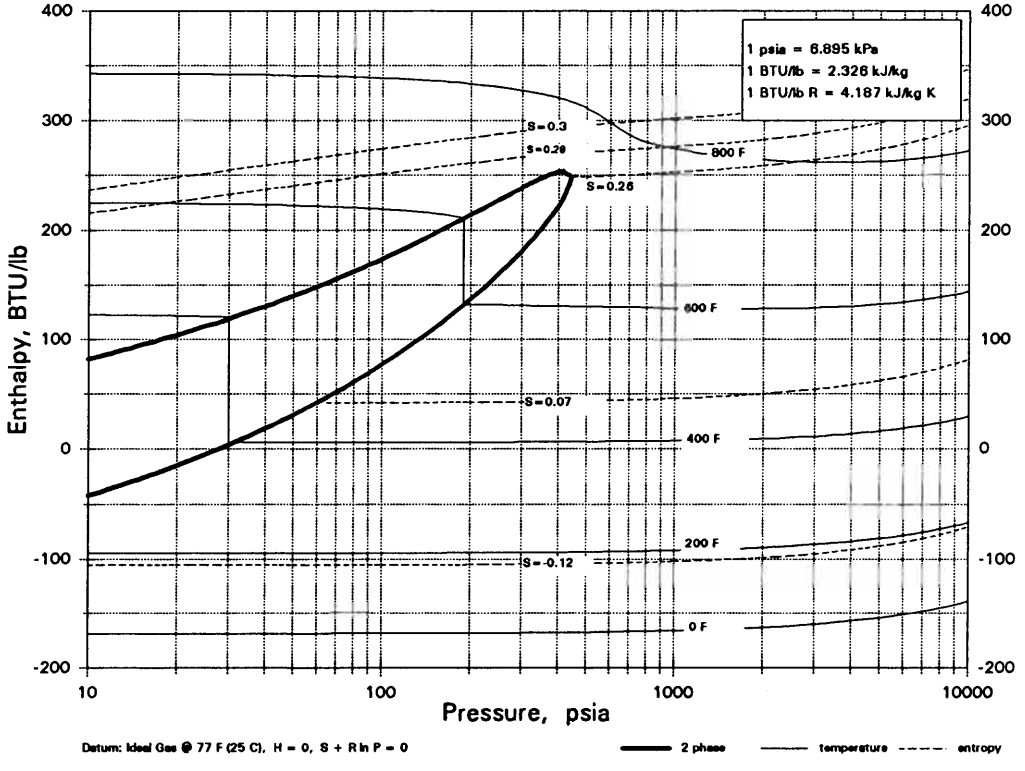
C10H10O4 DIMETHYL TEREPHTHALATE



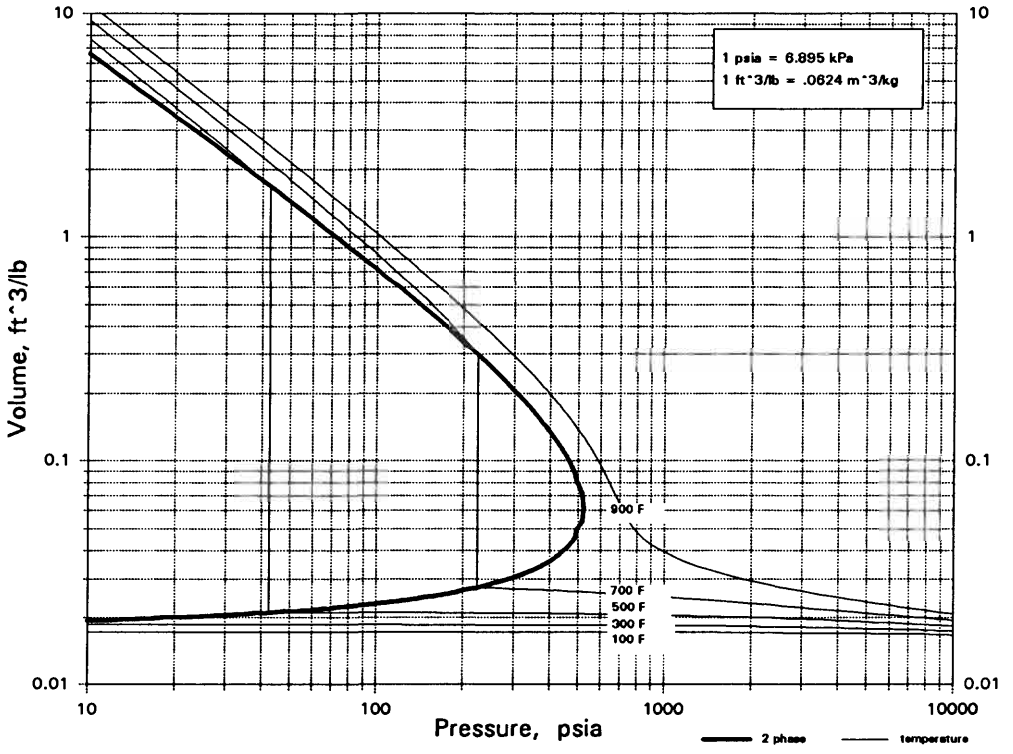


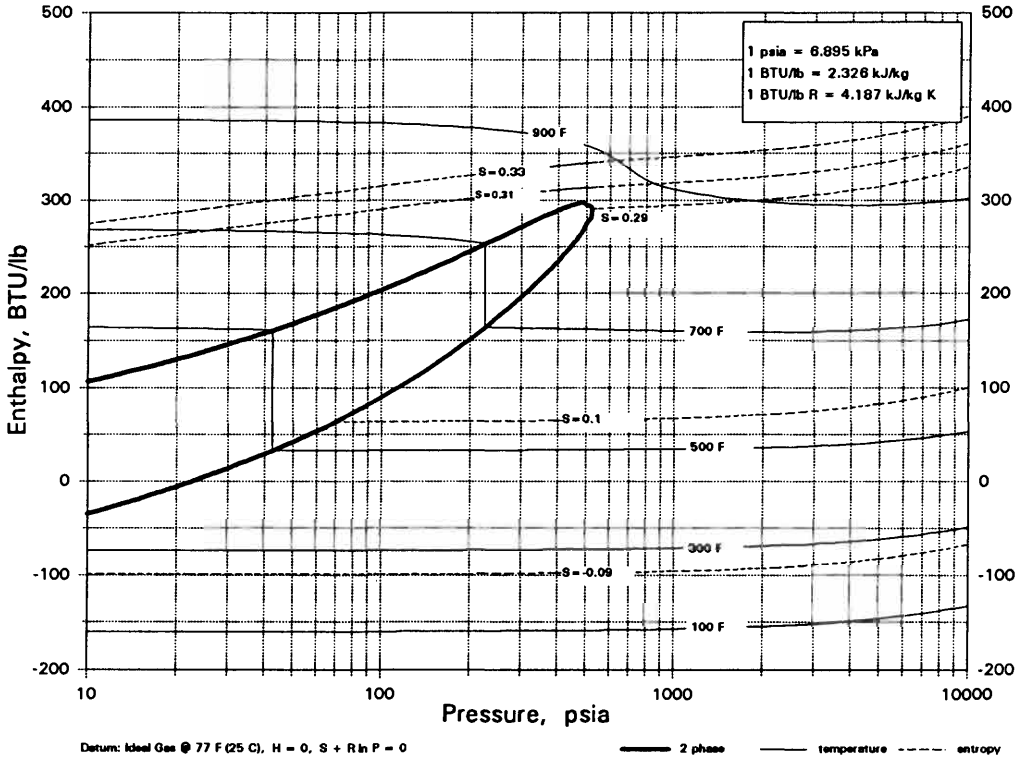
C10H12 DICYCLOPENTADIENE



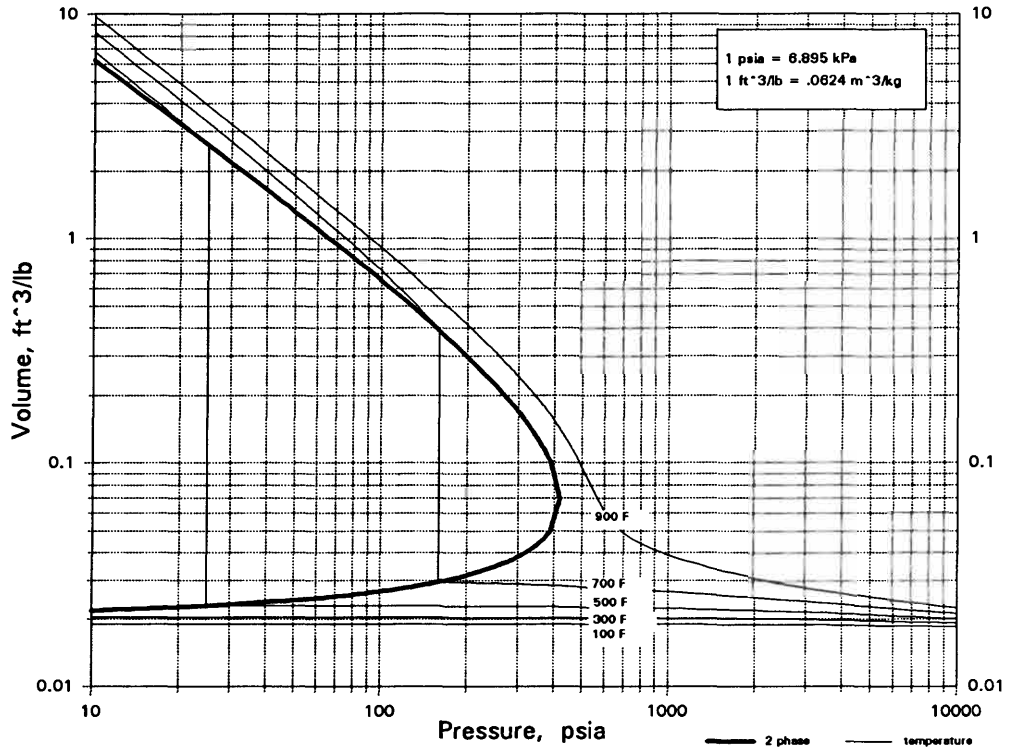


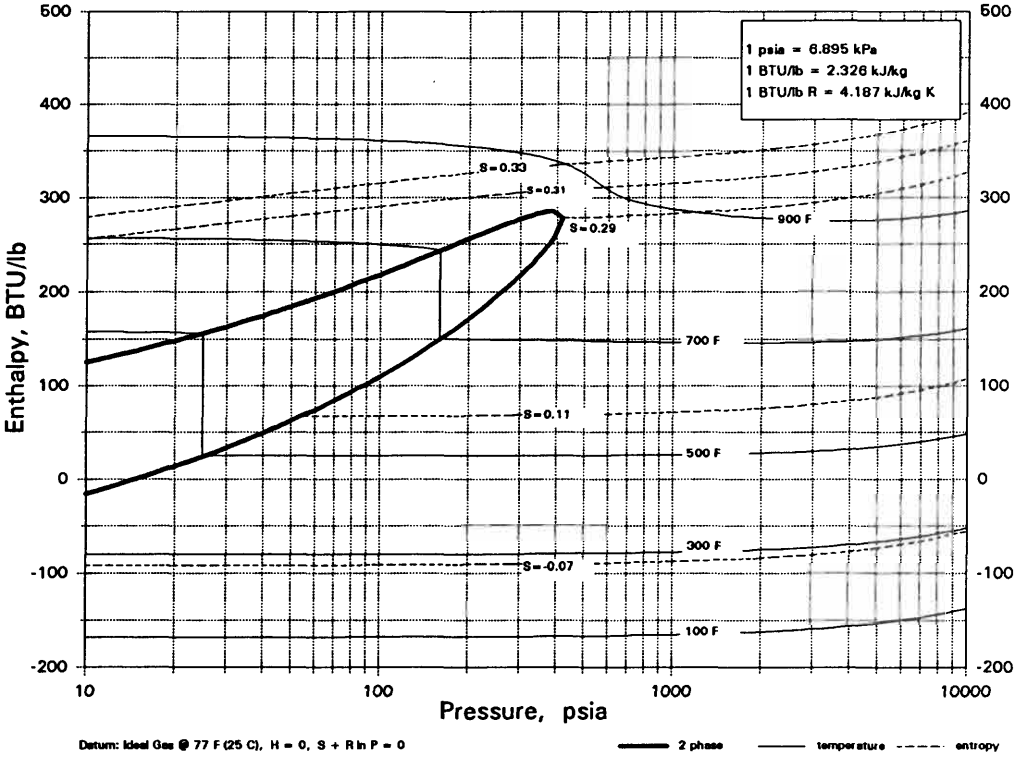
C10H12 1-2-3-4-TETRAHYDRONAPHTHALENE



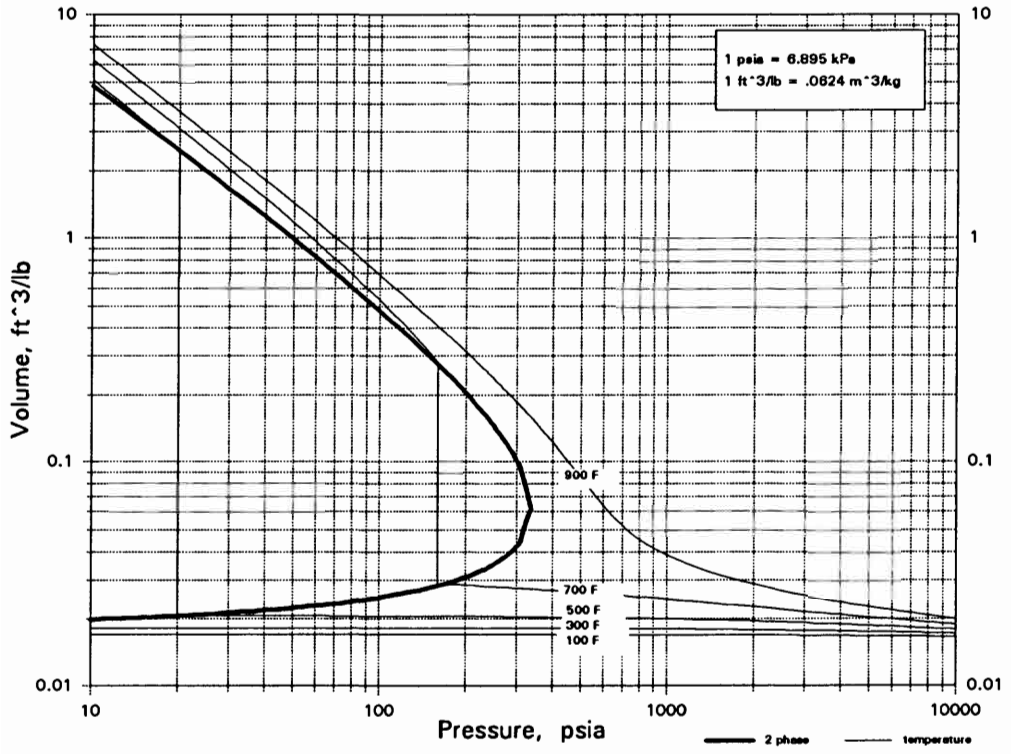


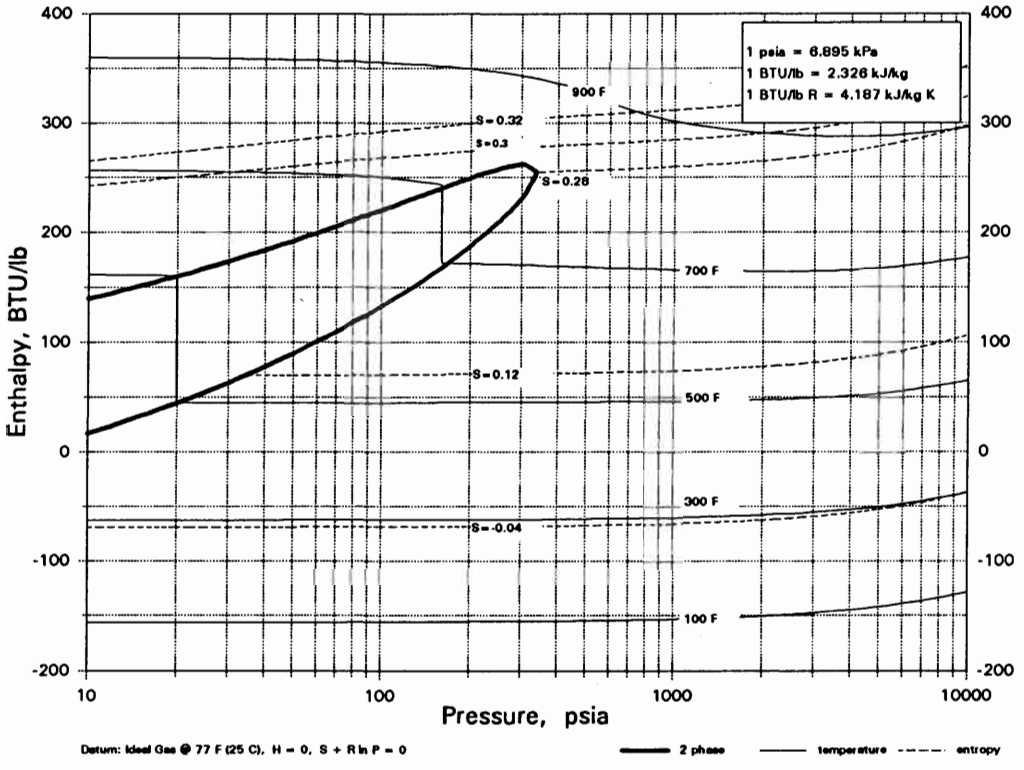
C10H12O ANETHOLE



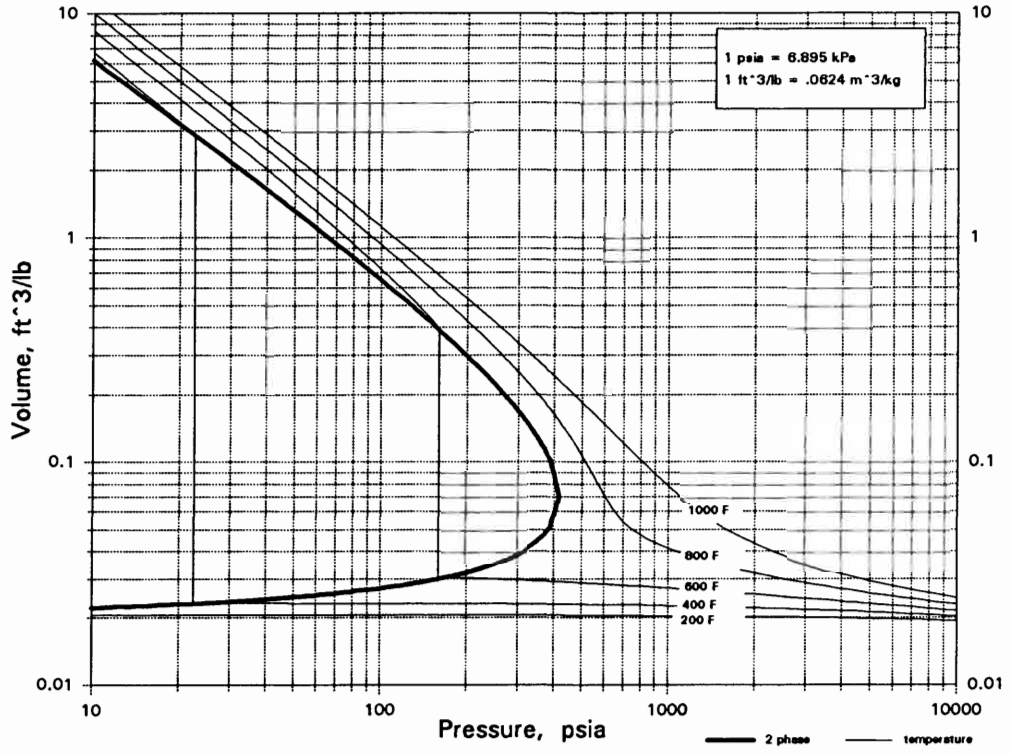


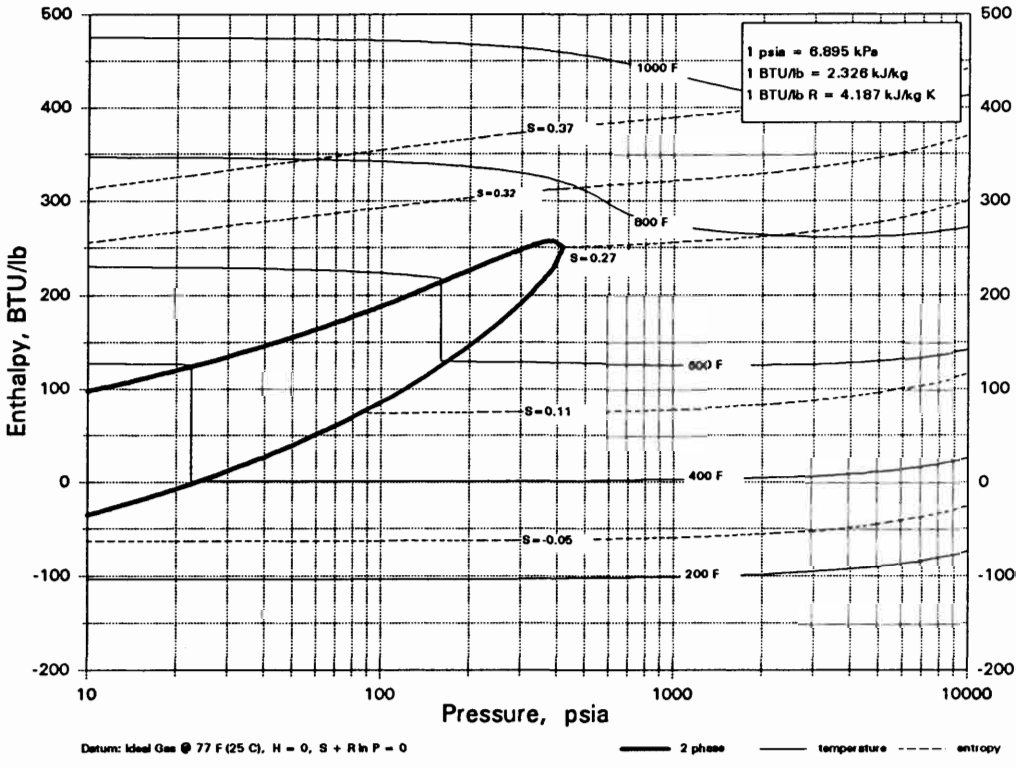
C10H12O4 DIALLYL MALEATE



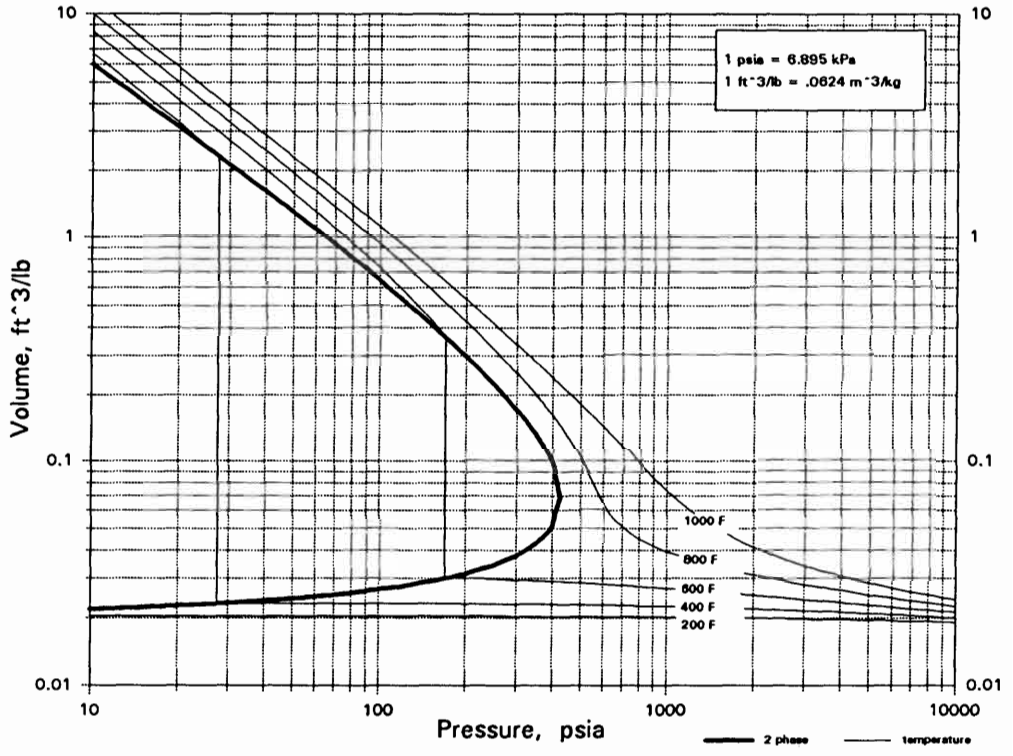


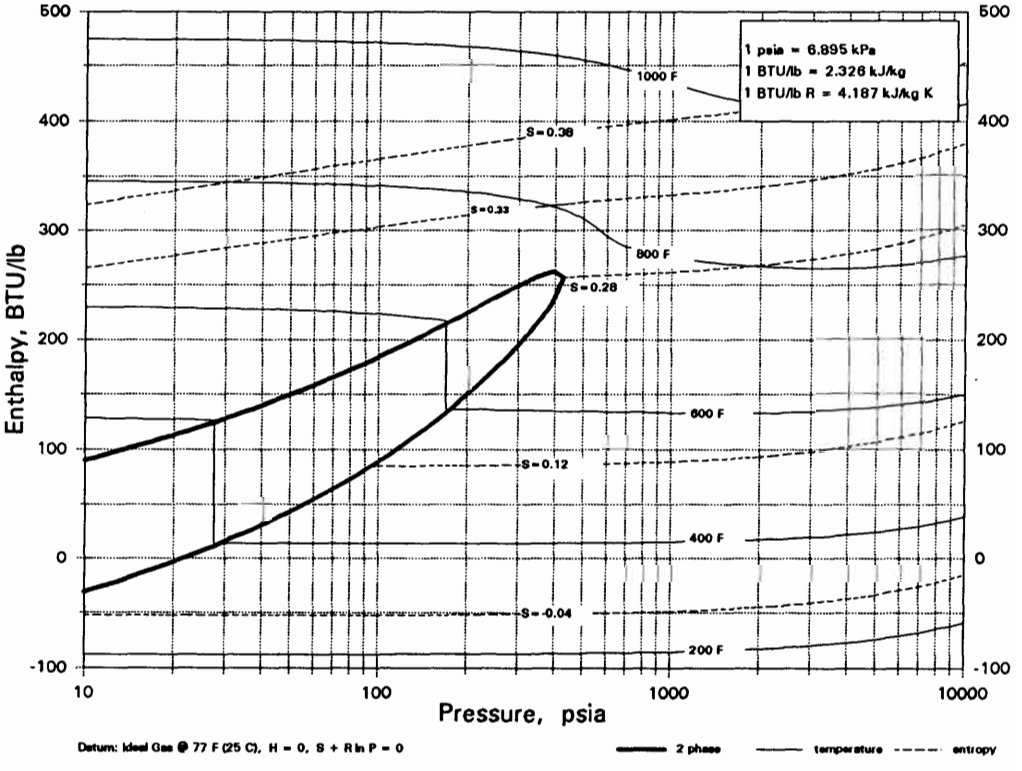
C10H14 n-BUTYLBENZENE



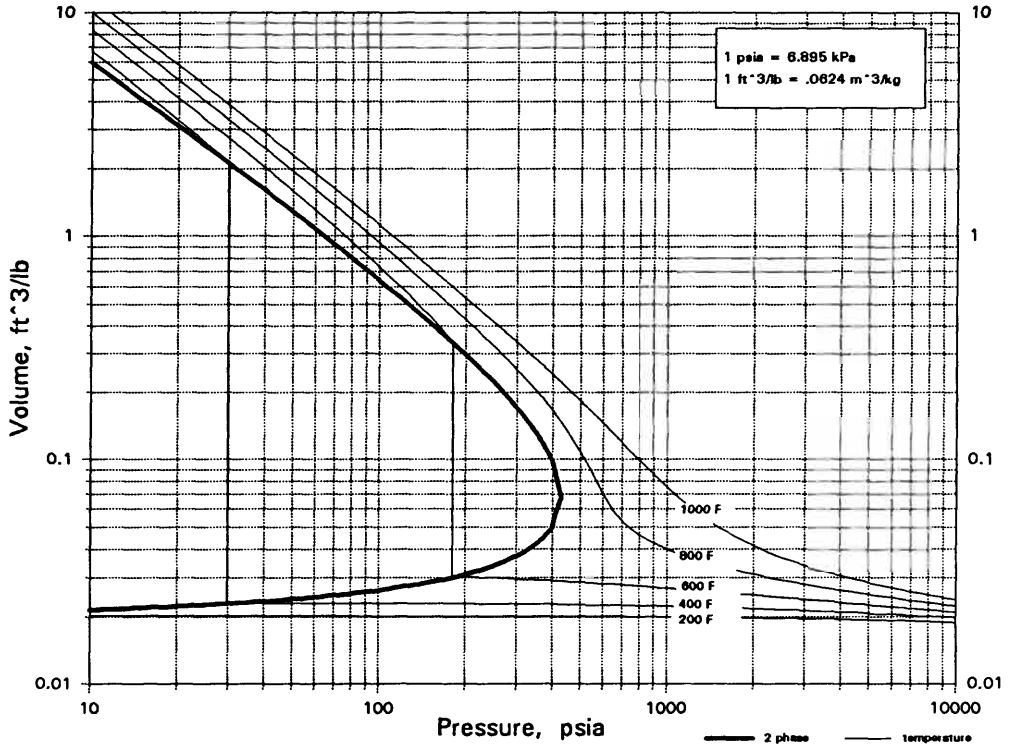


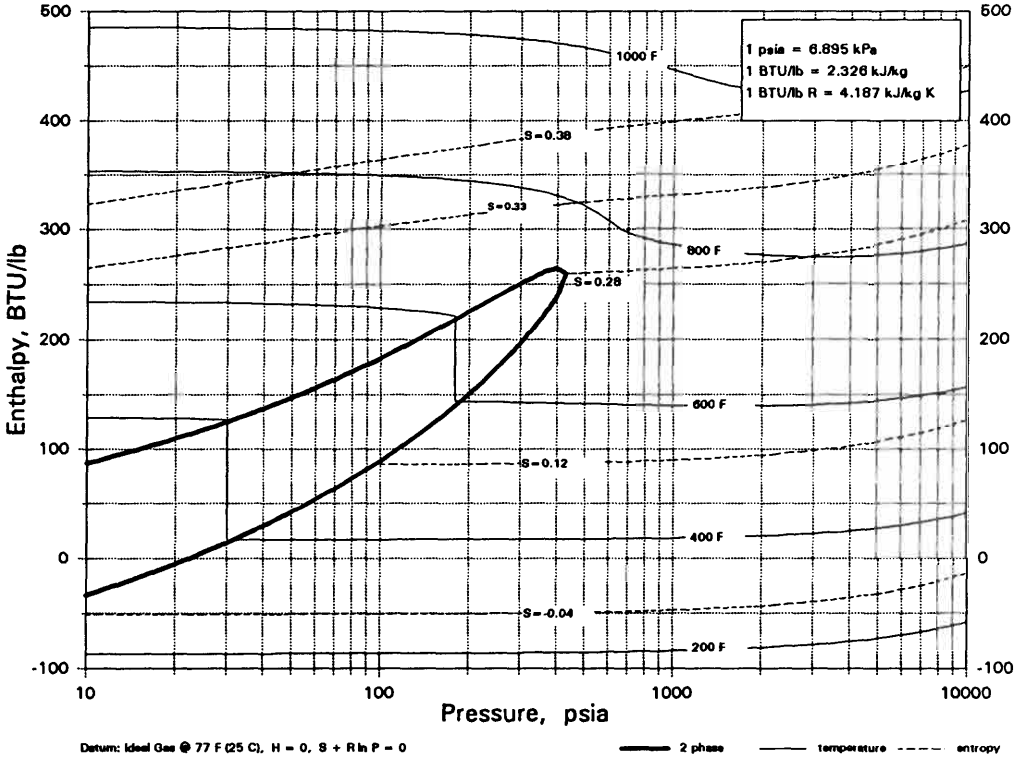
C10H14 sec-BUTYLBENZENE



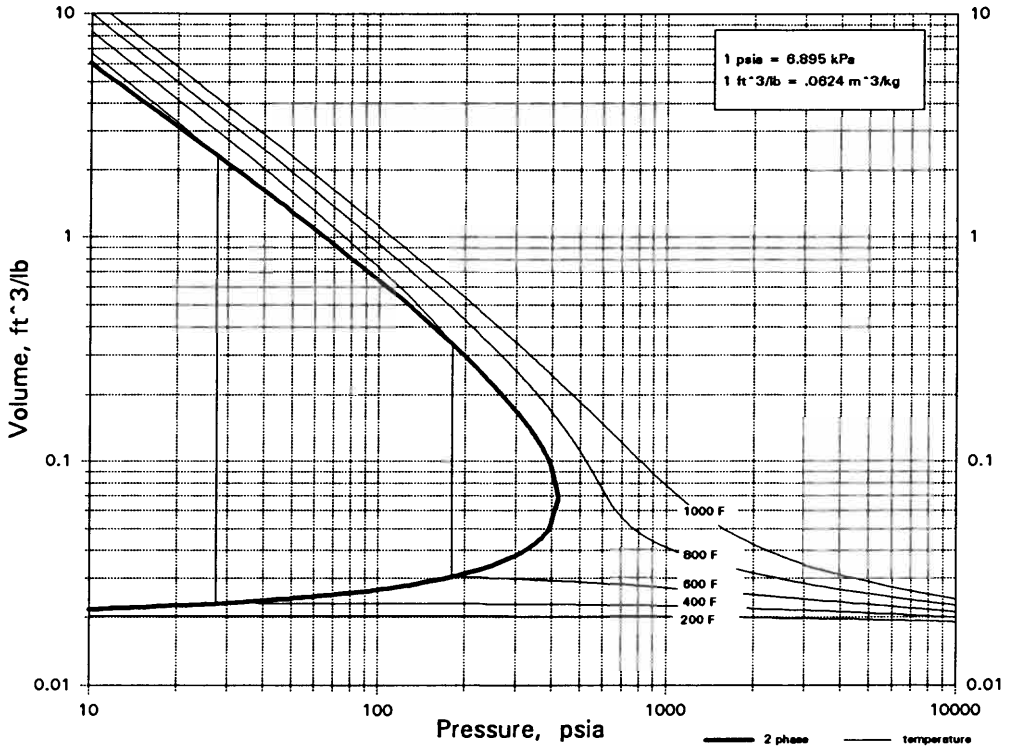


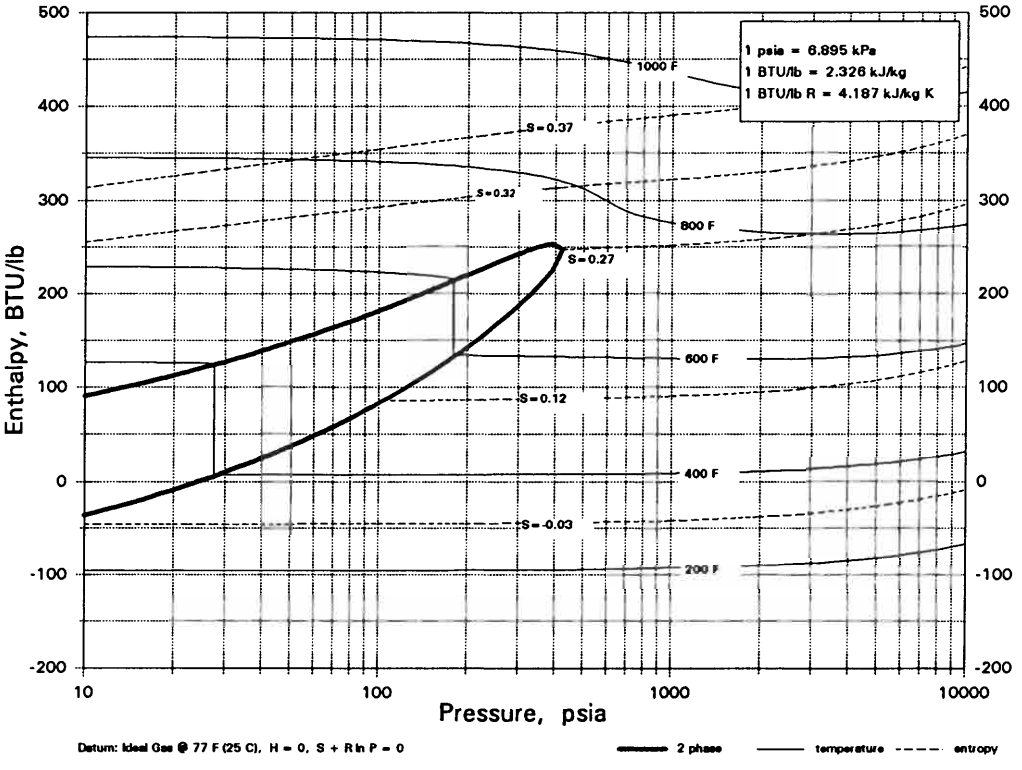
C10H14 tert-BUTYLBENZENE



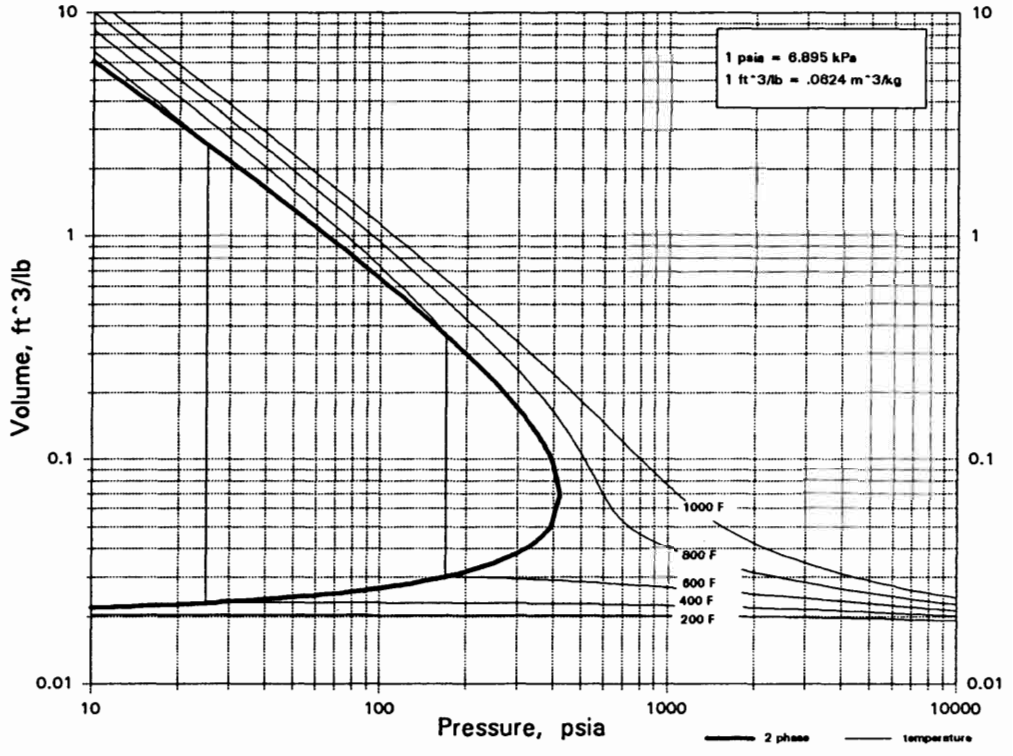


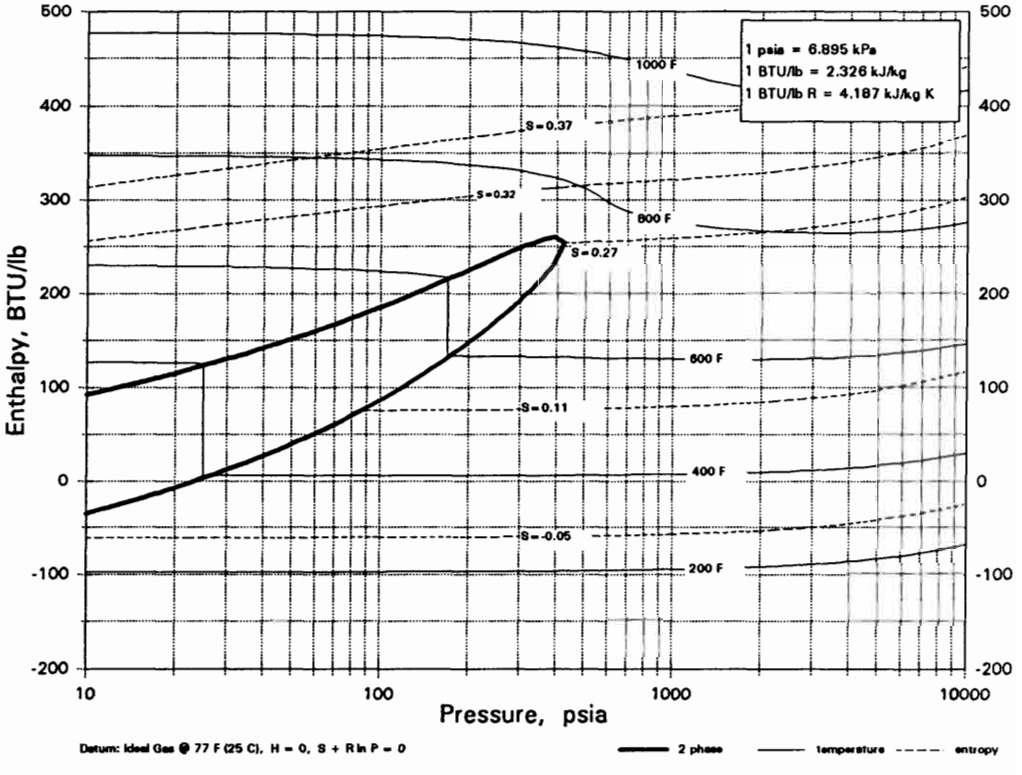
C10H14 m-CYMENE



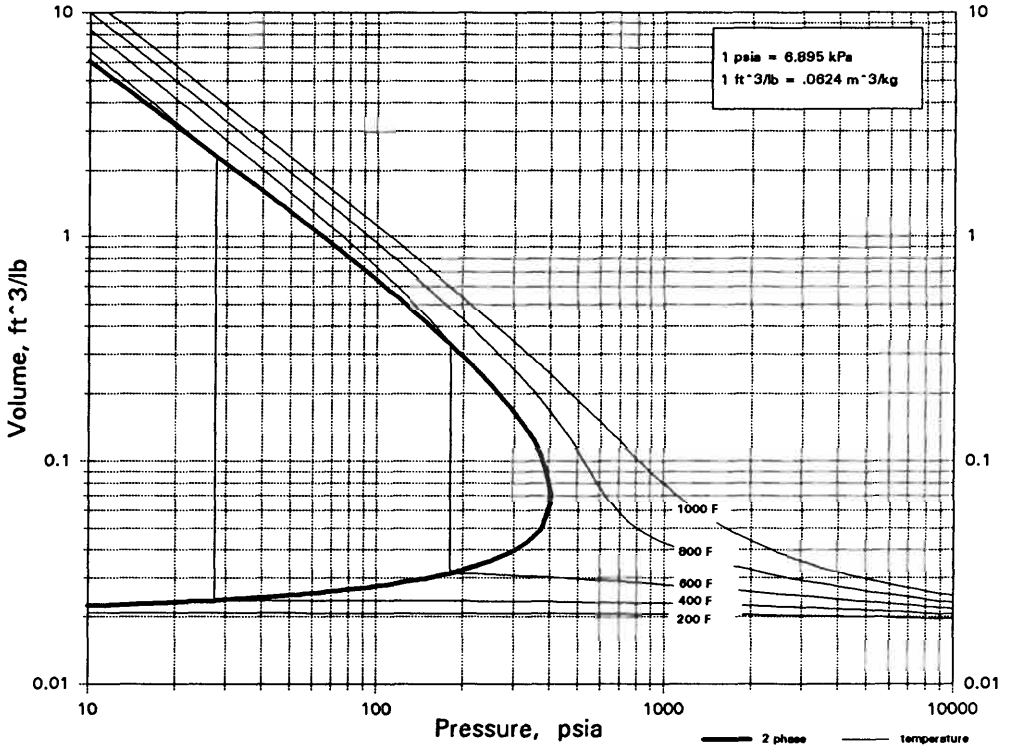


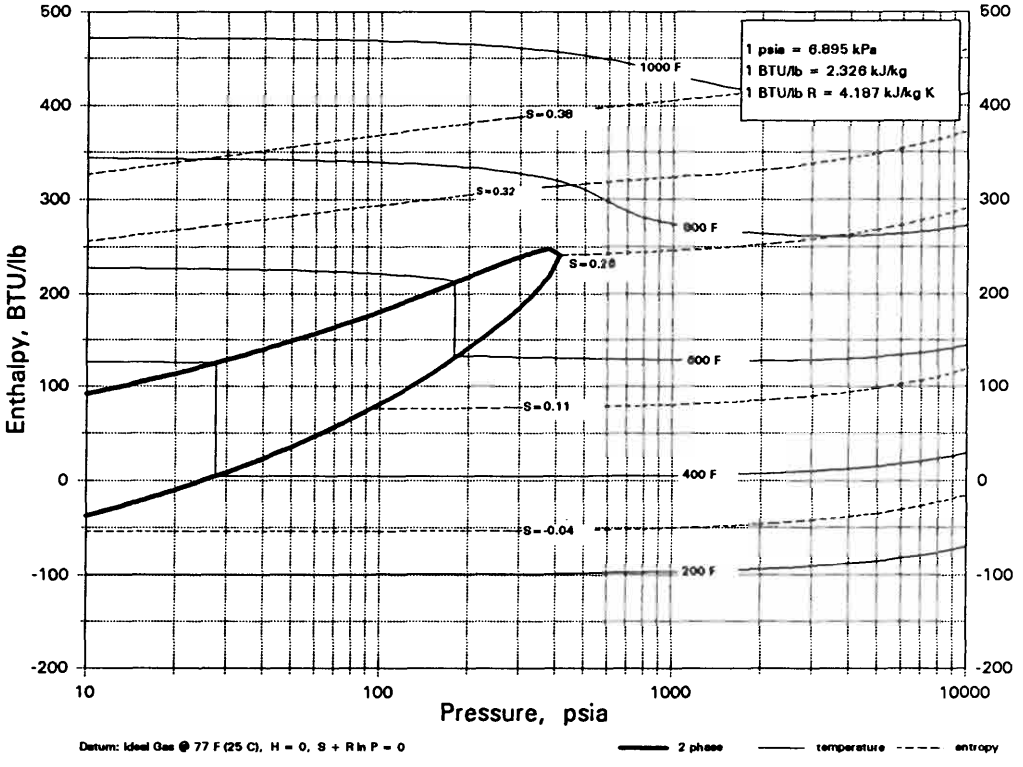
C10H14 o-CYMENE





C10H14 p-CYMENE





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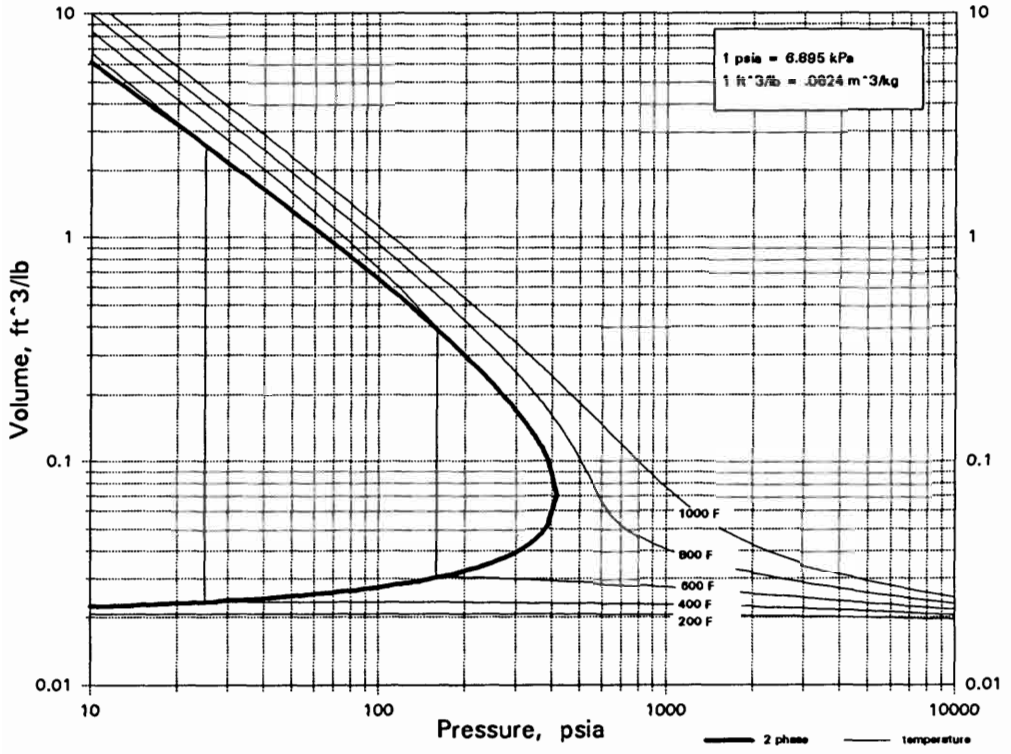
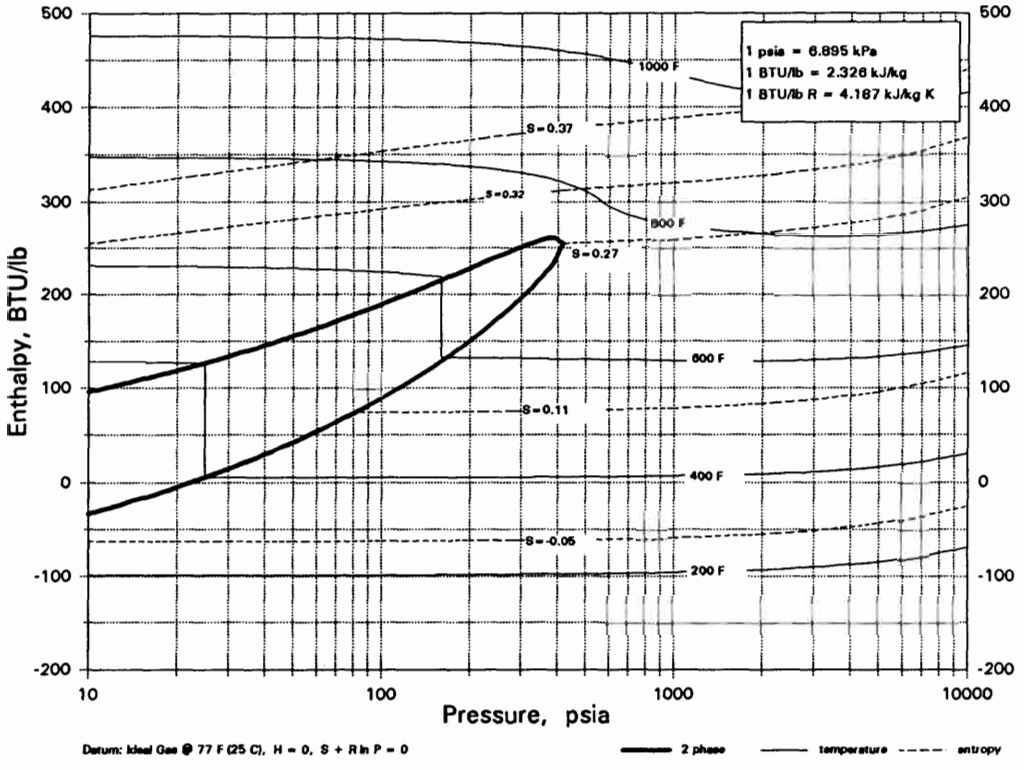
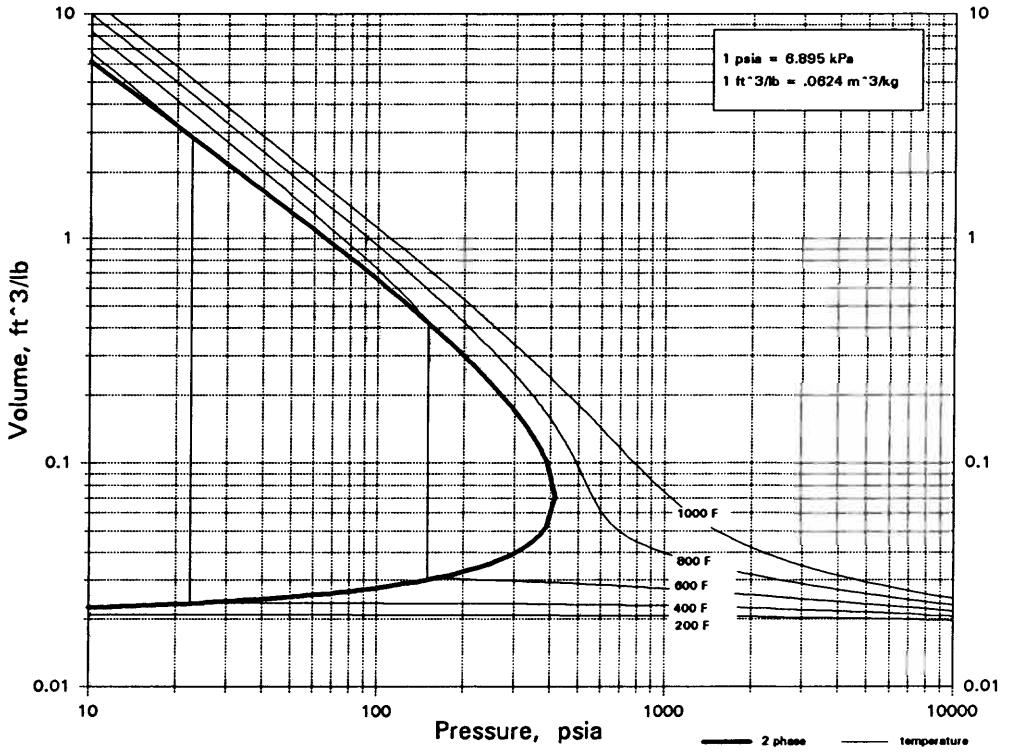
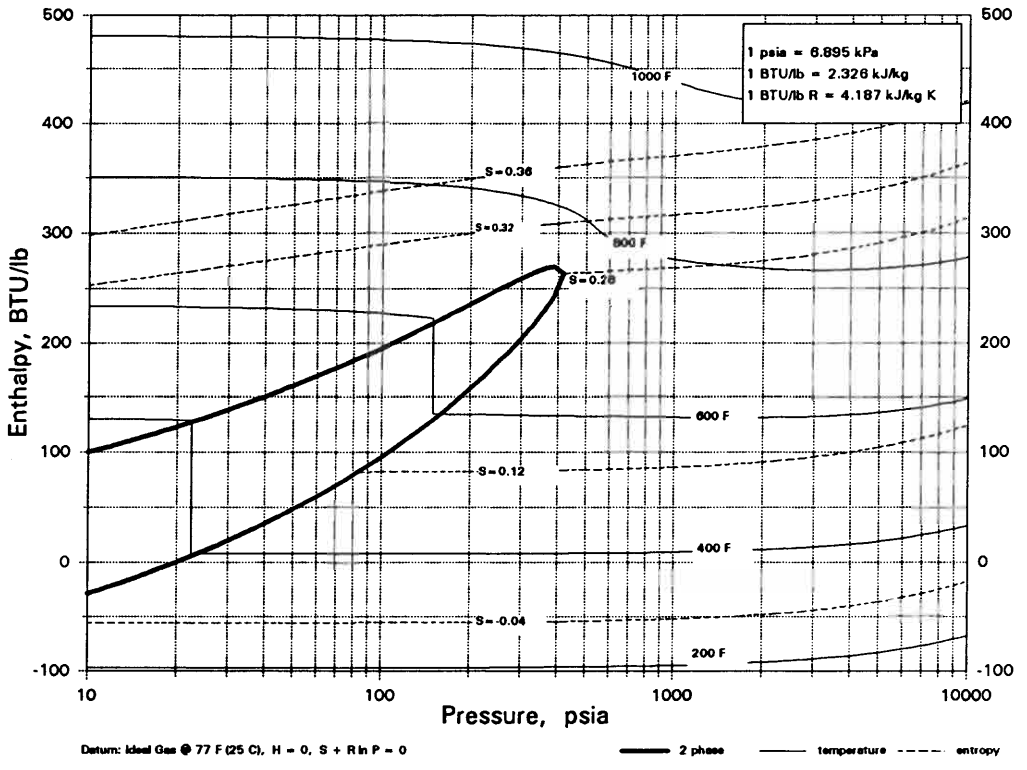




C10H14 o-DIETHYLBENZENE





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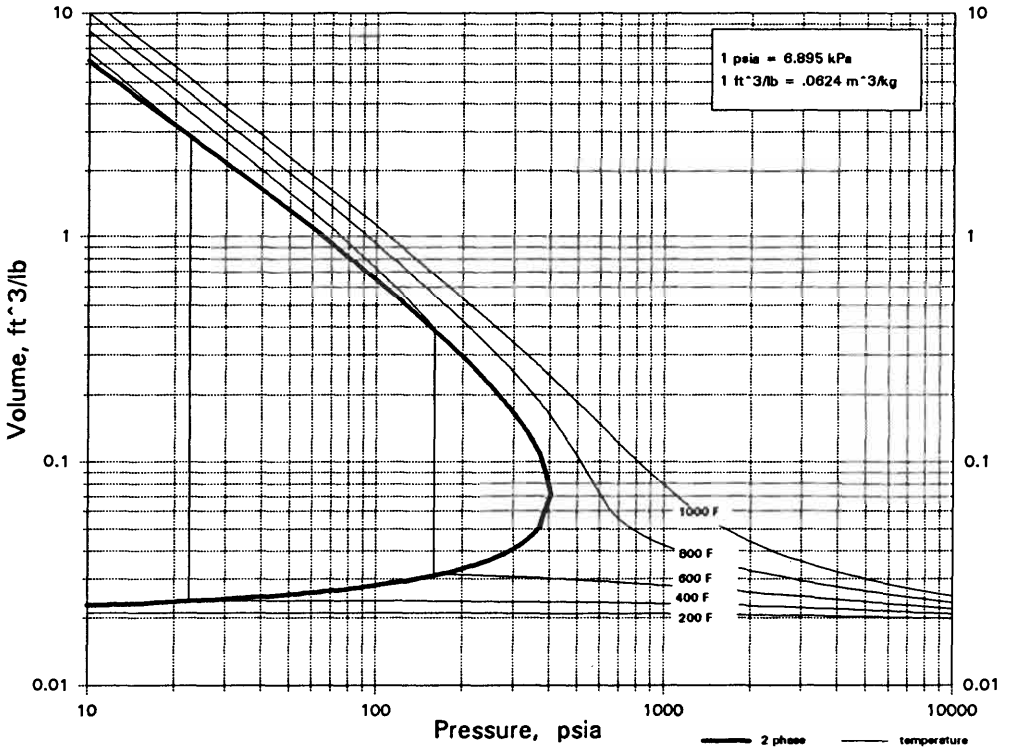
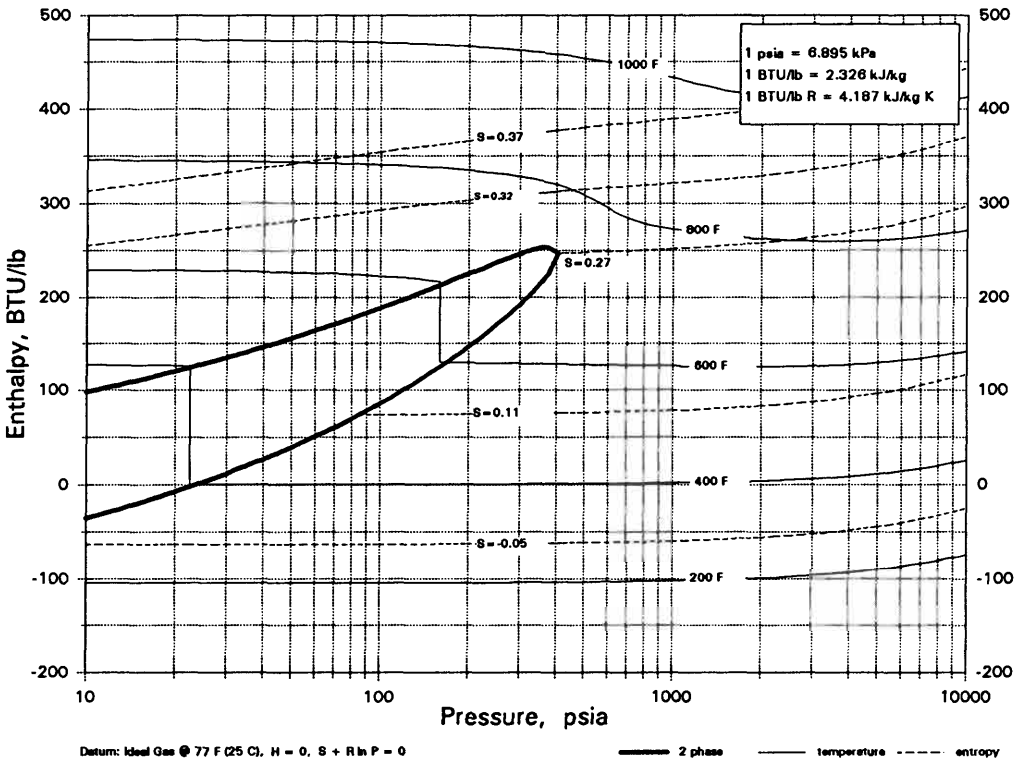
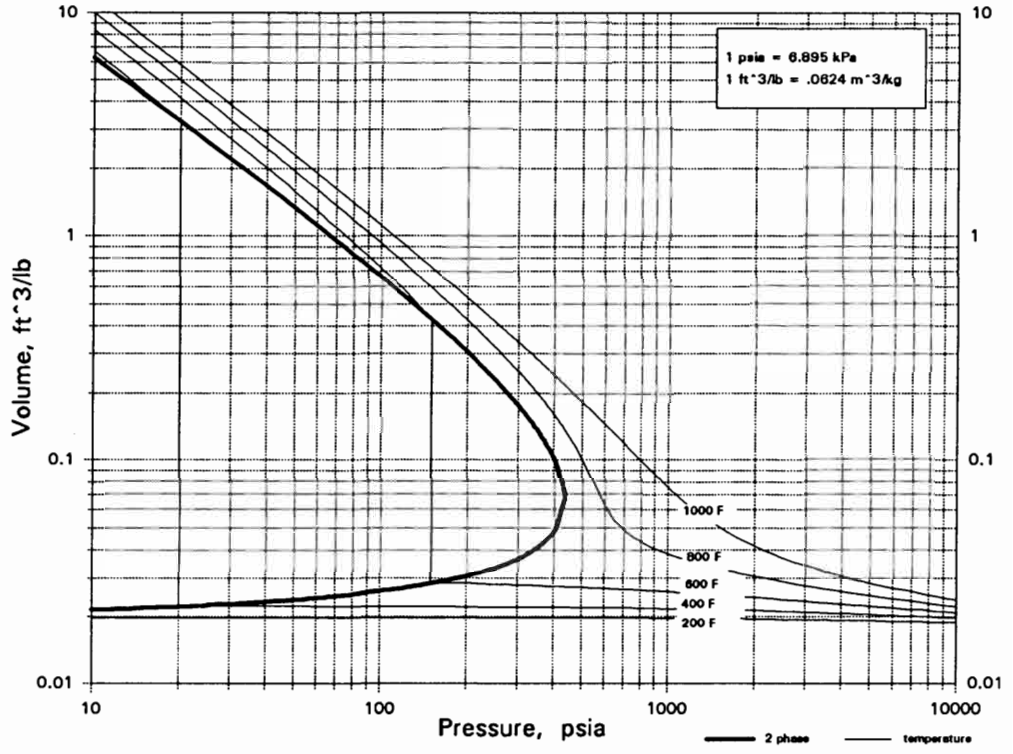
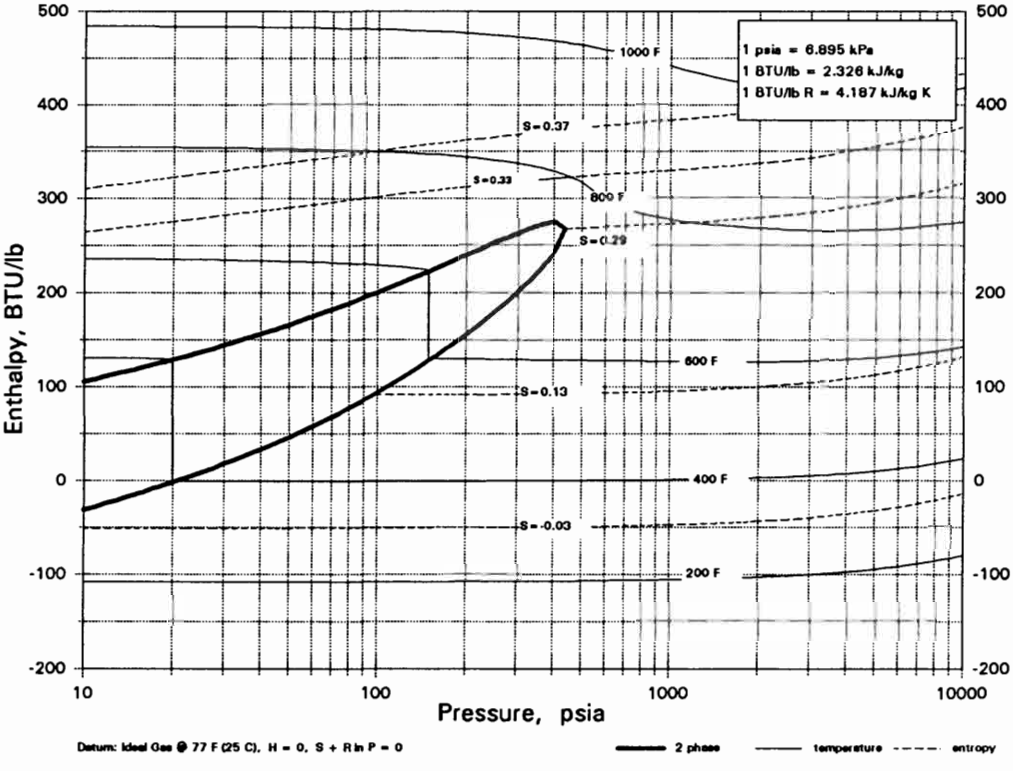




C1OH14 2-ETHYL-m-XYLENE





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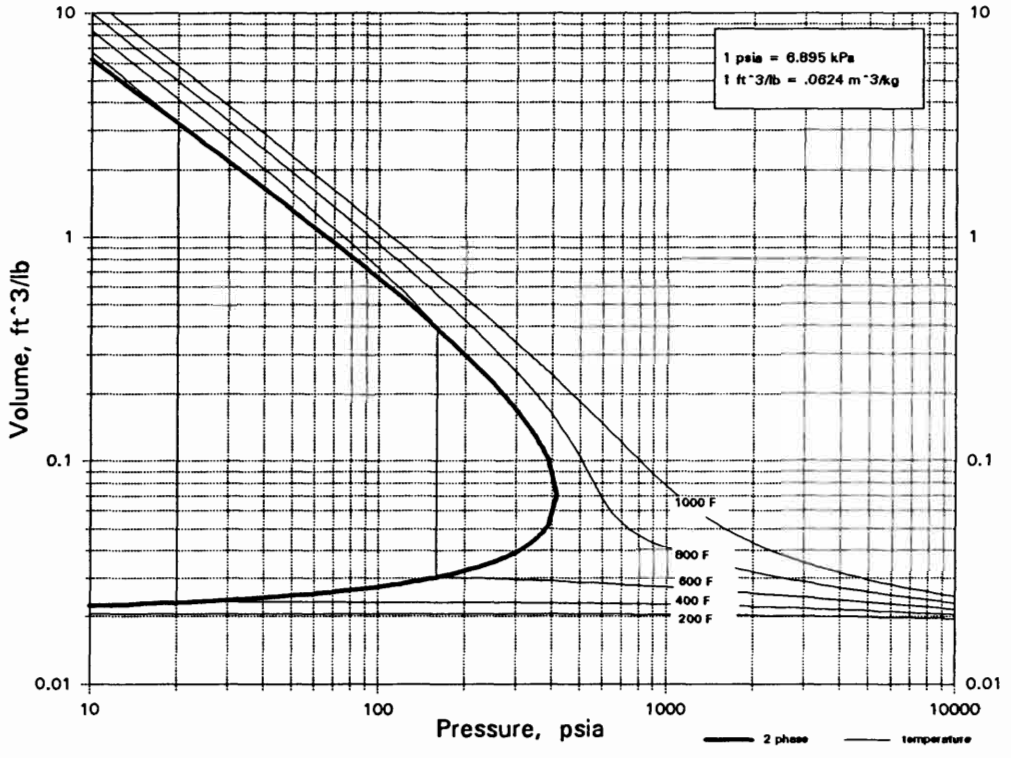
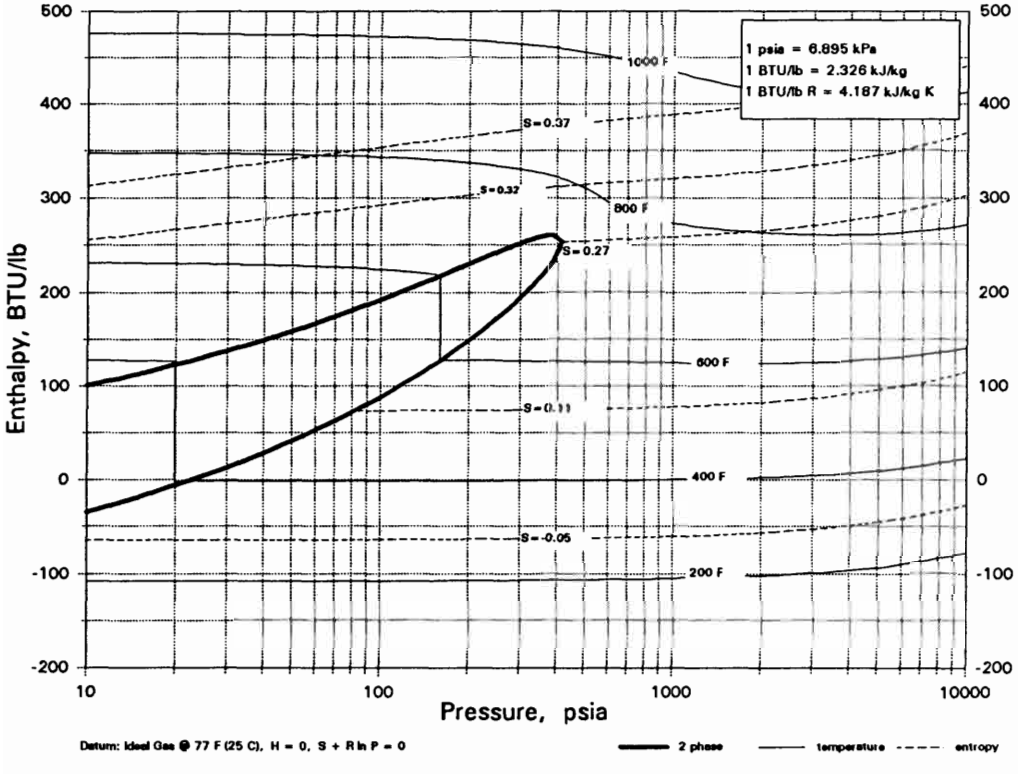
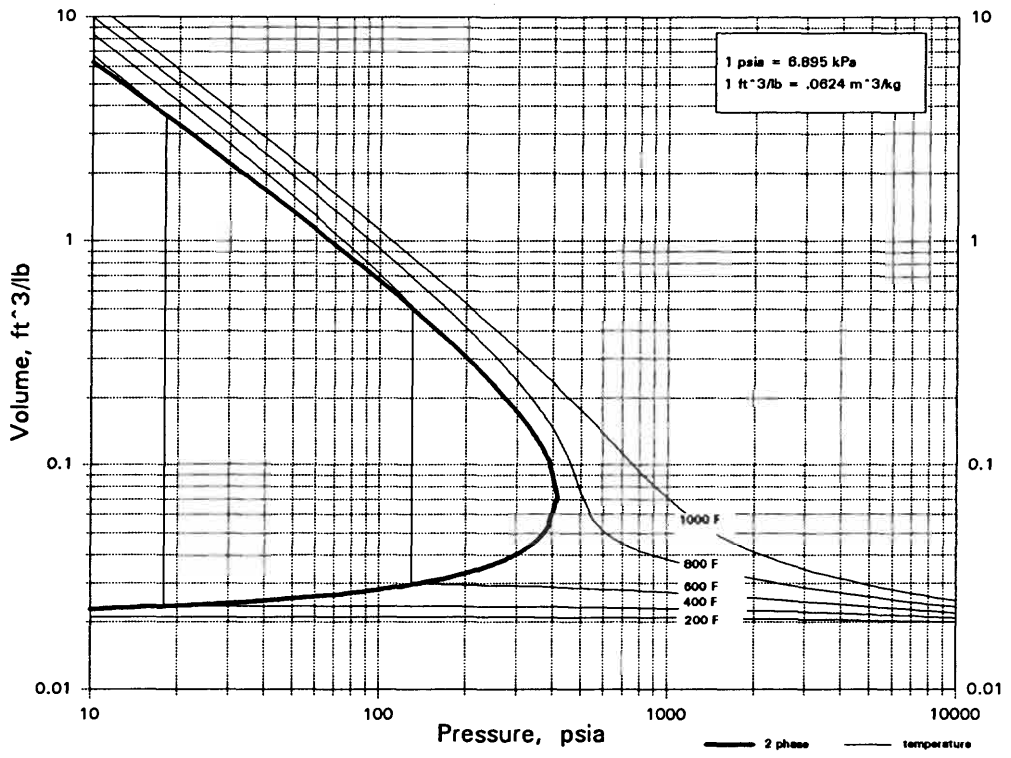
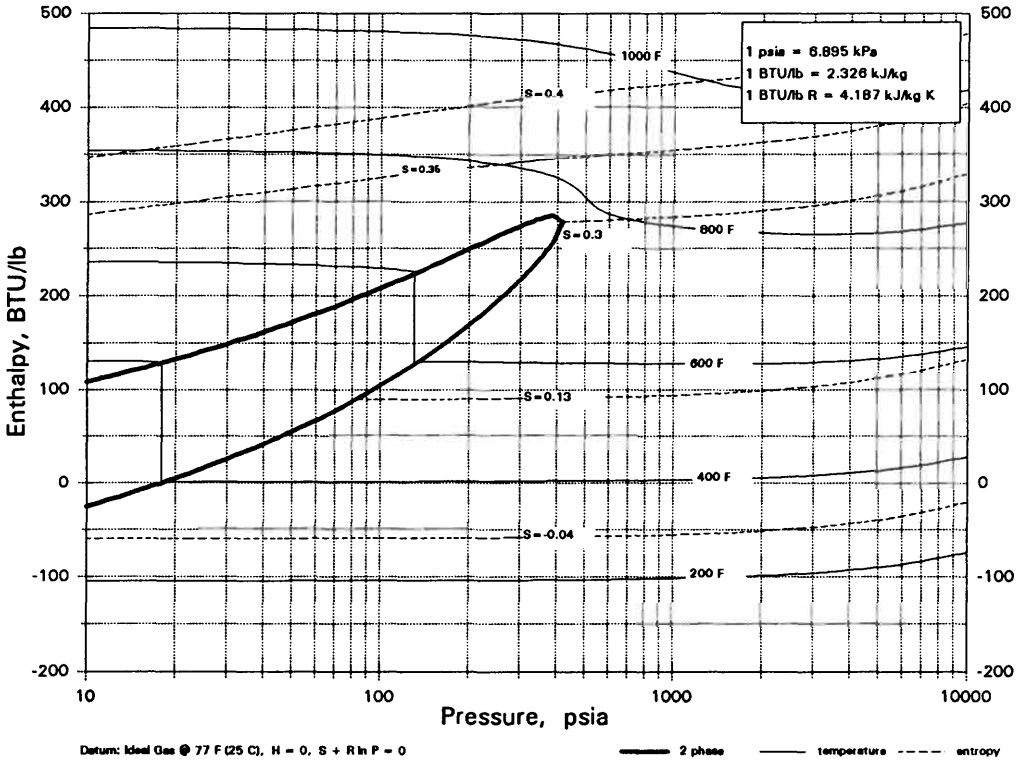


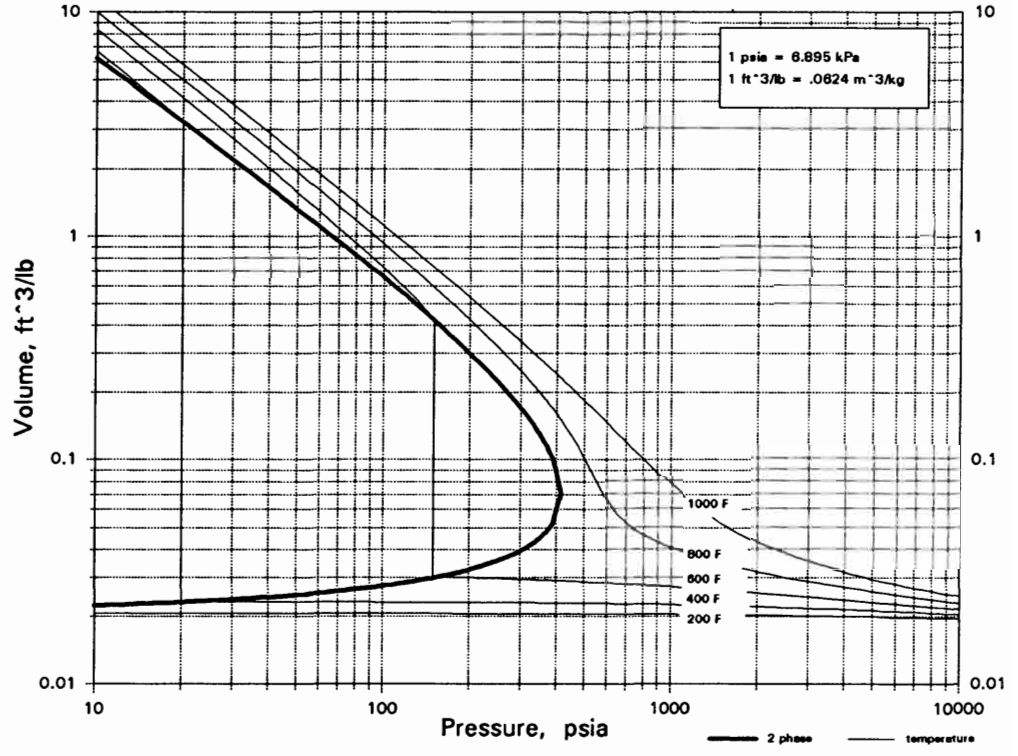


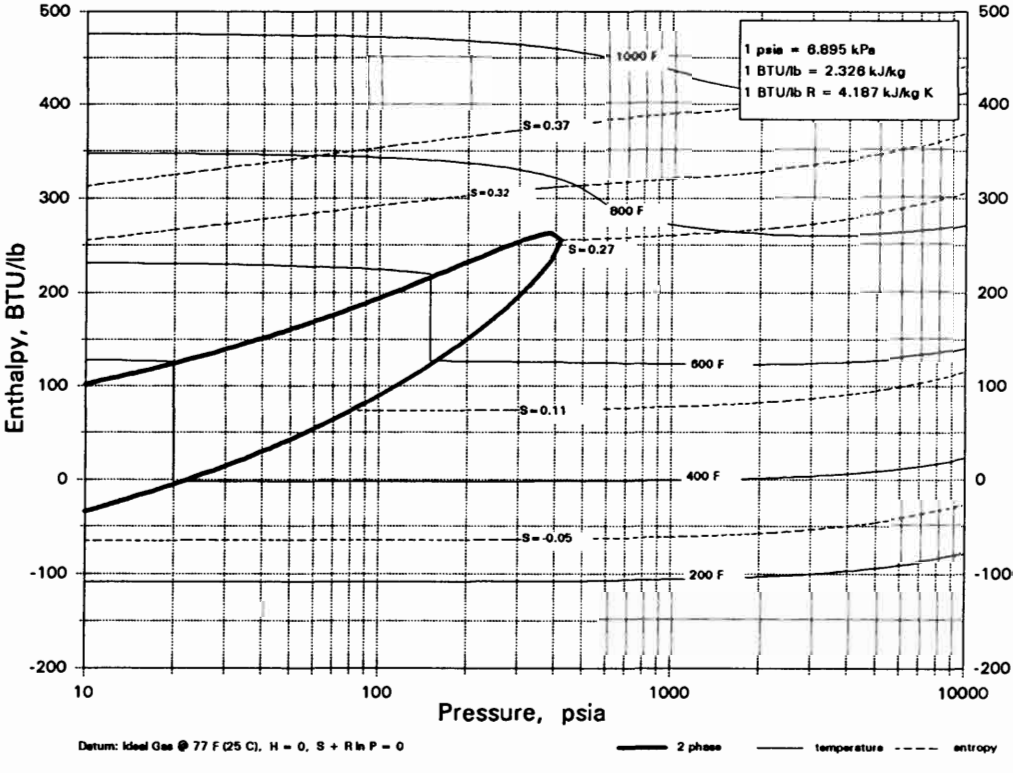
C10H14 3-ETHYL-o-XYLENE



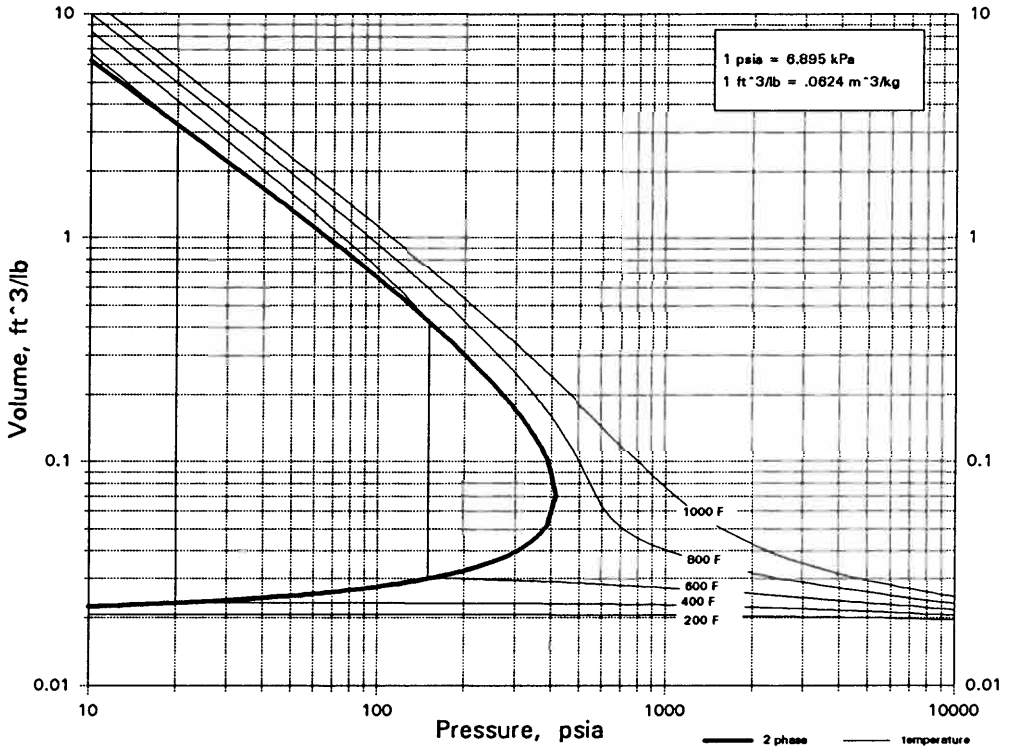


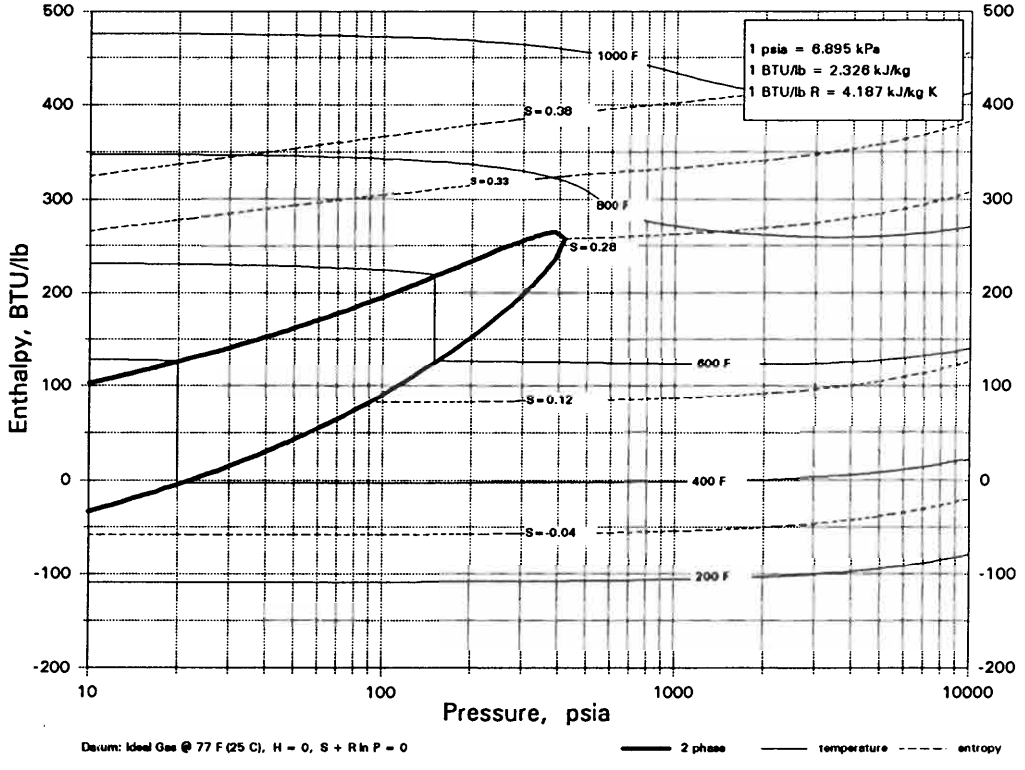
C10H14 4-ETHYL-m-XYLENE



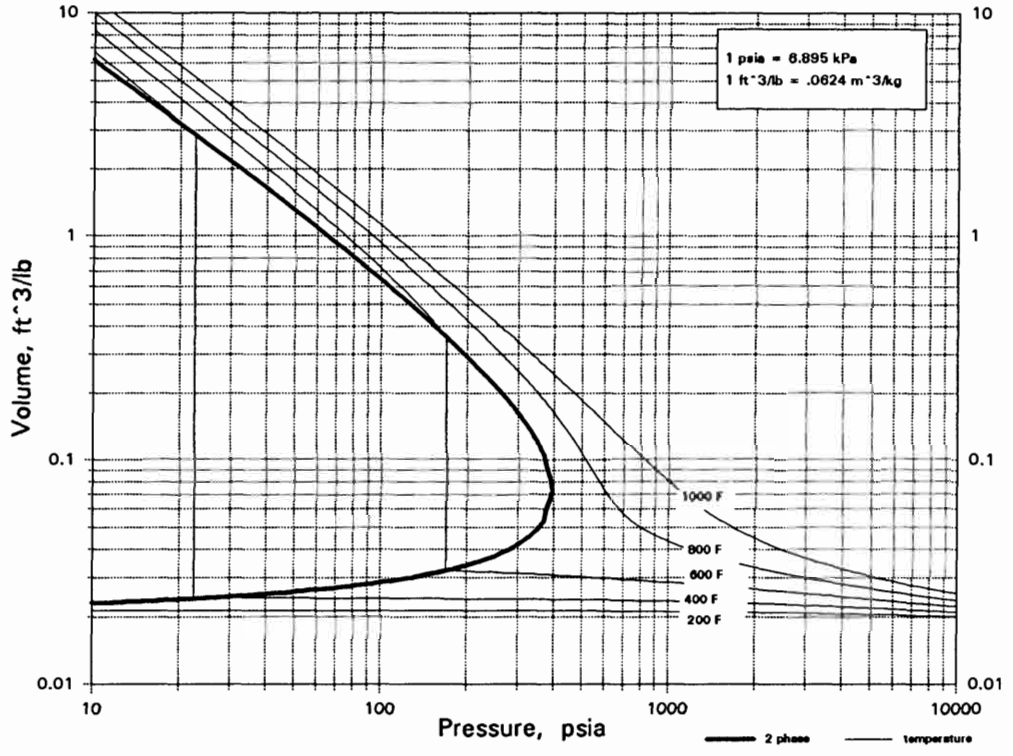


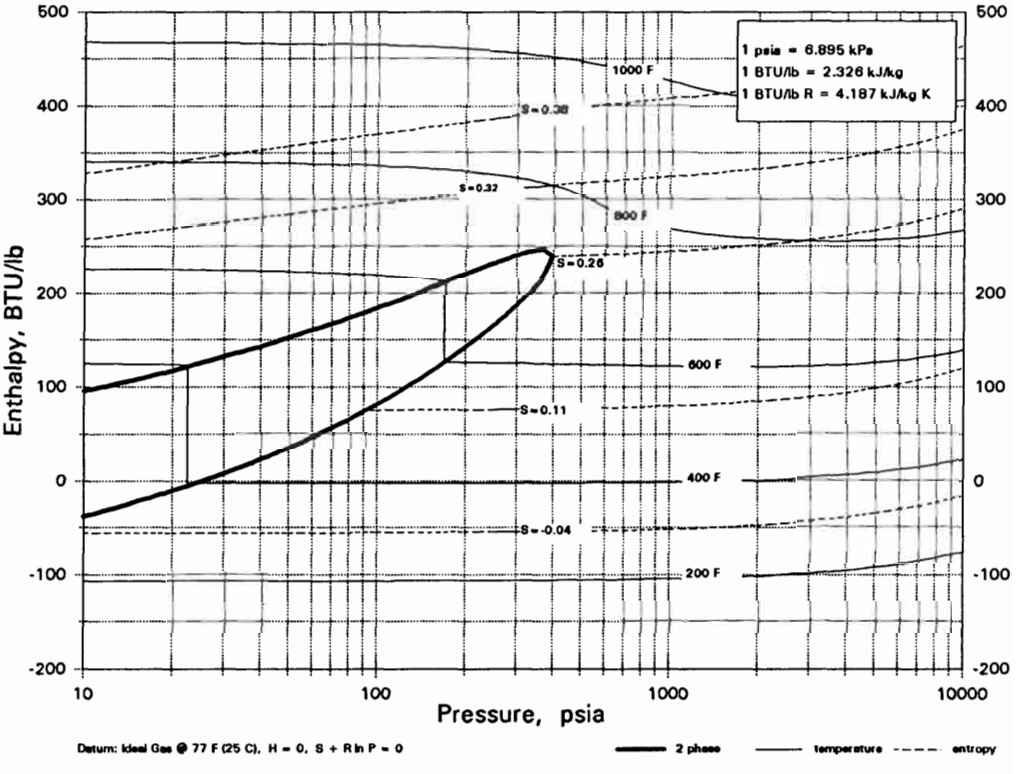
C10H14 4-ETHYL-o-XYLENE



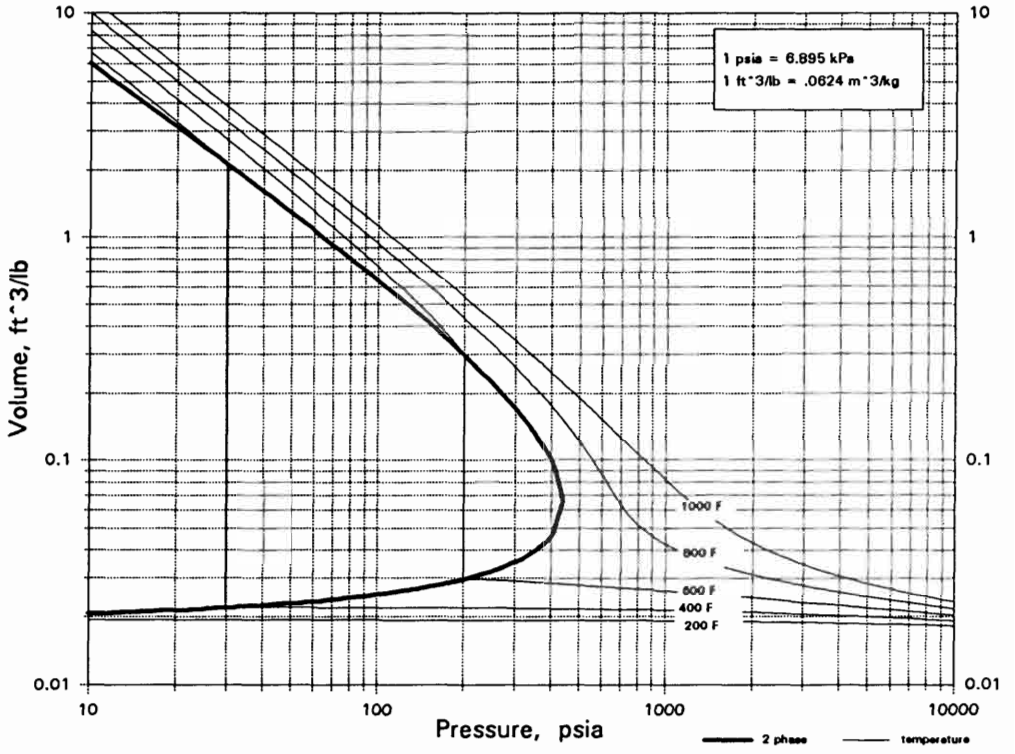


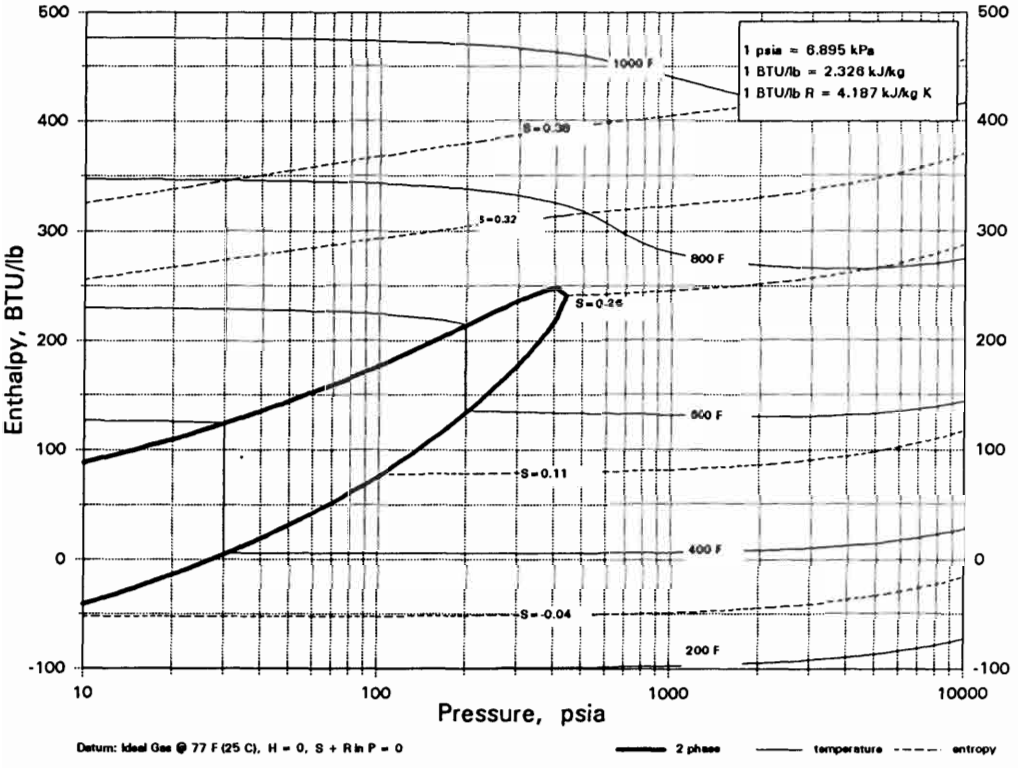
C10H14 5-ETHYL-m-XYLENE



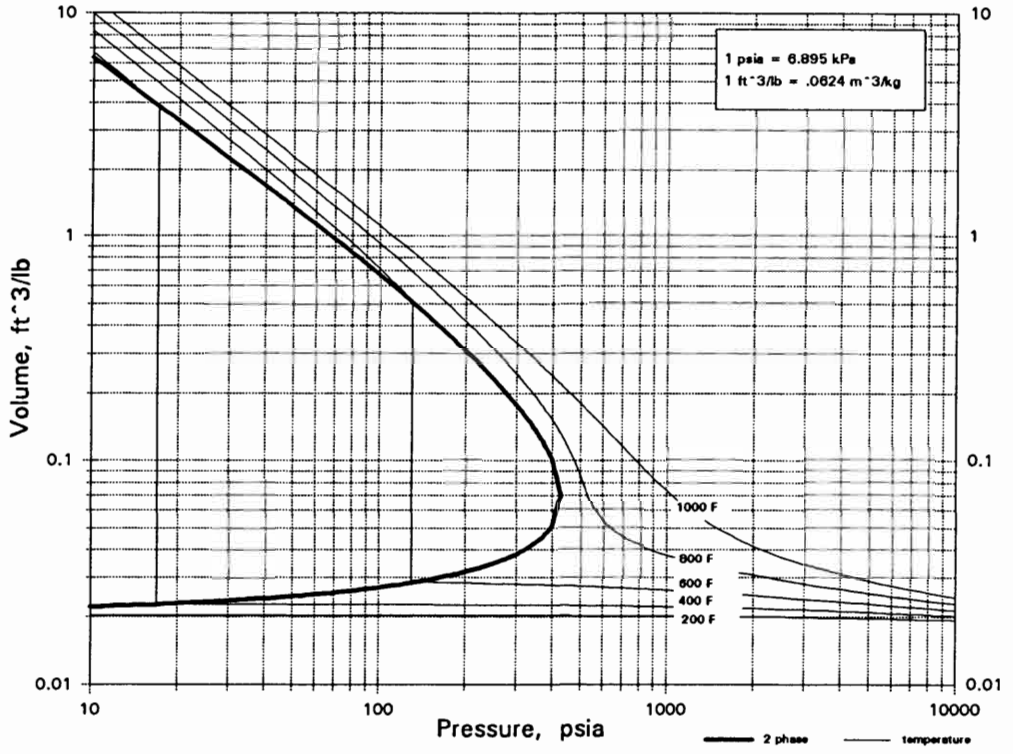


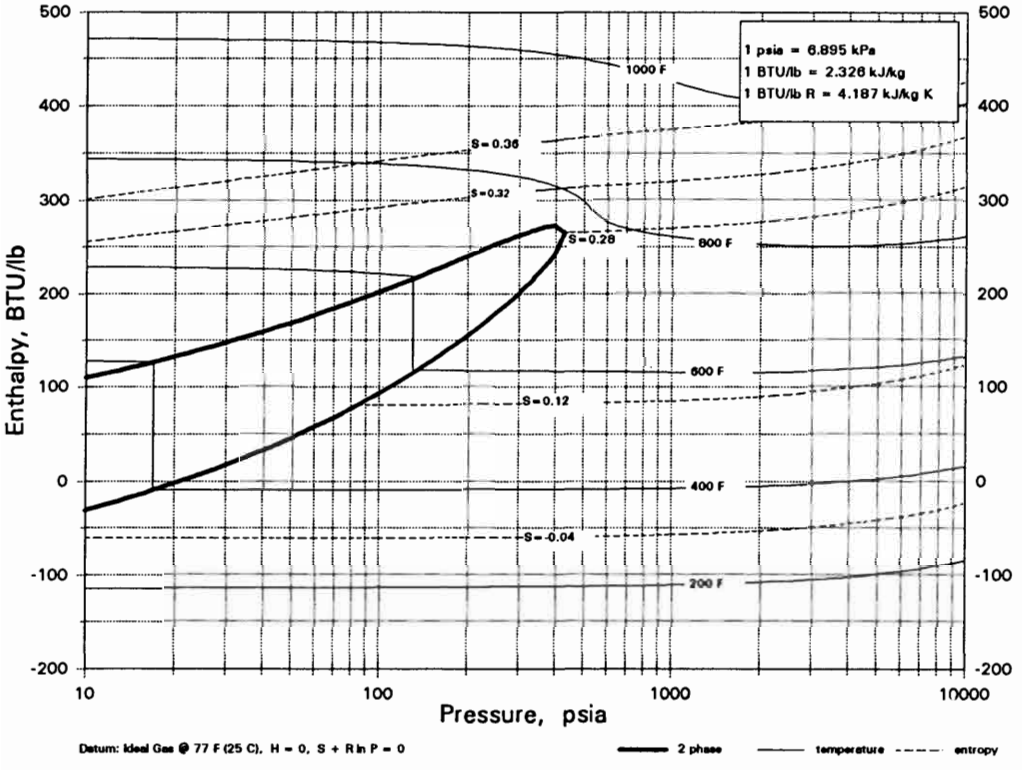
C10H14 ISOBUTYLBENZENE



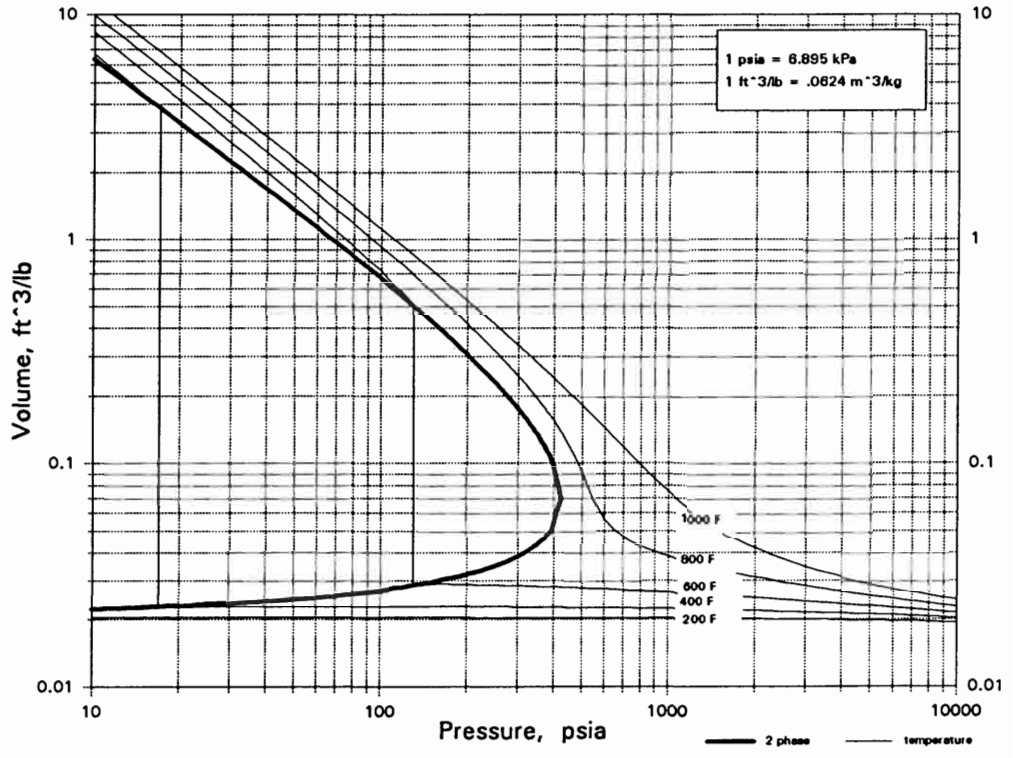


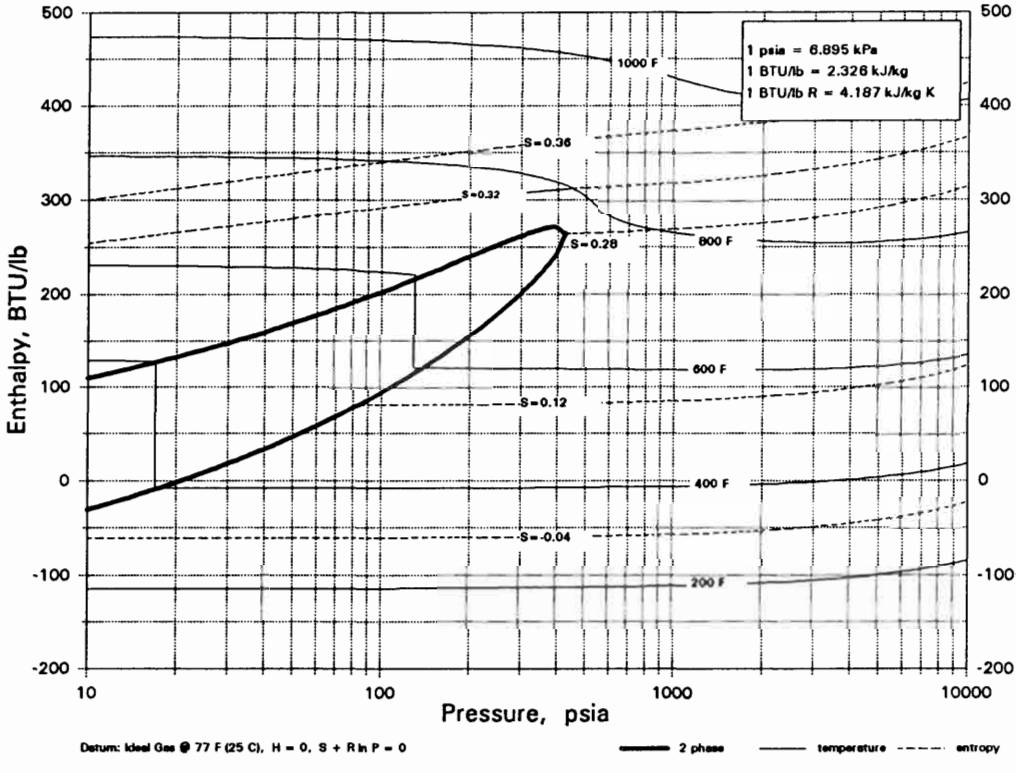
C10H14 1-2-3-5-TETRAMETHYLBENZENE



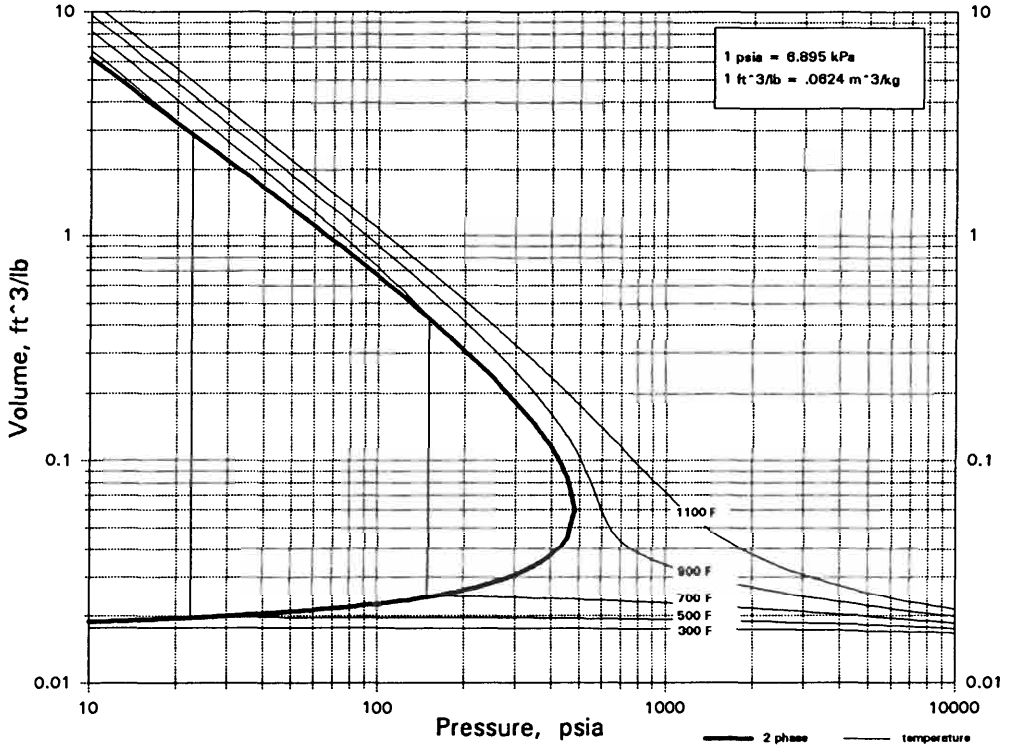


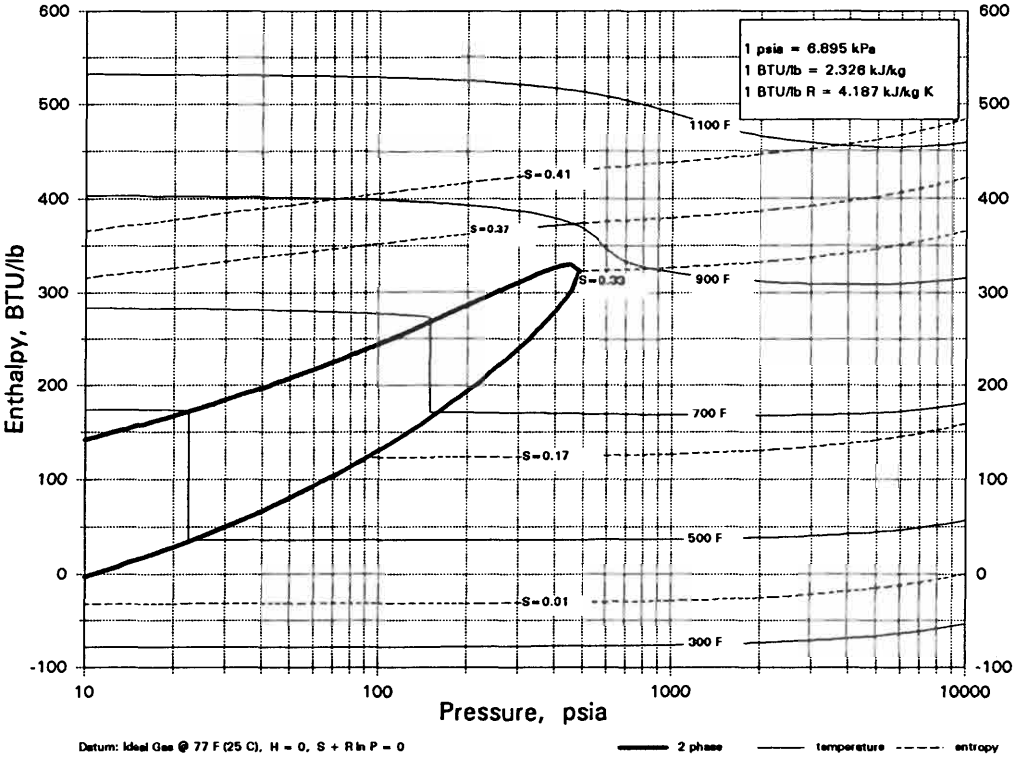
C10H14 1-2-4-5-TETRAMETHYLBENZENE



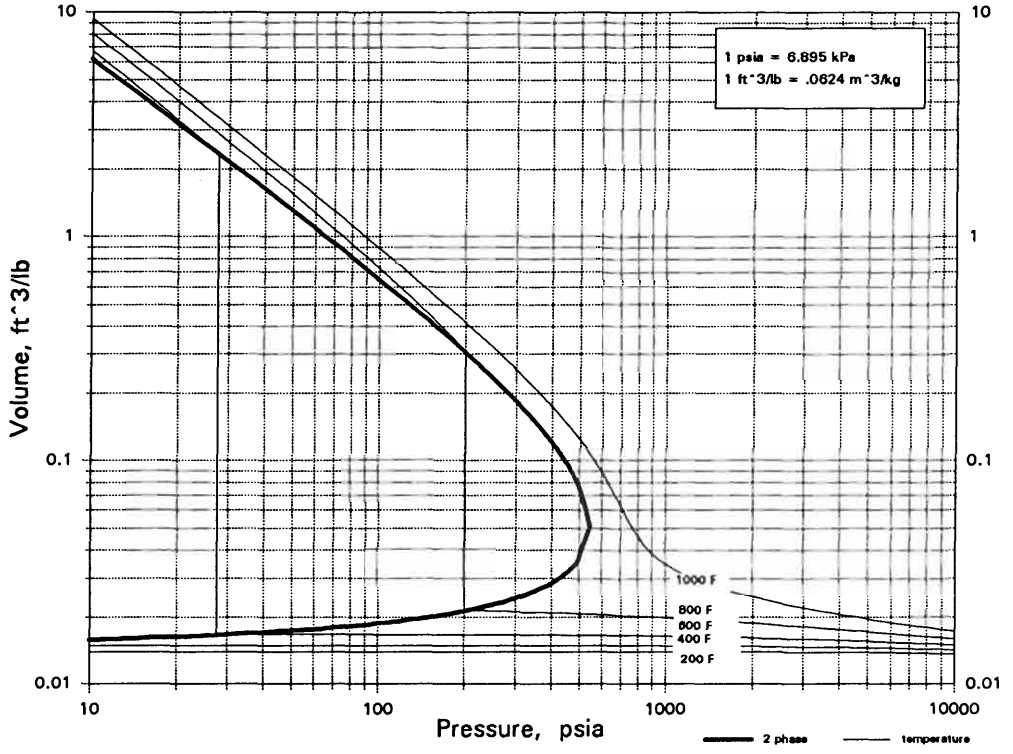


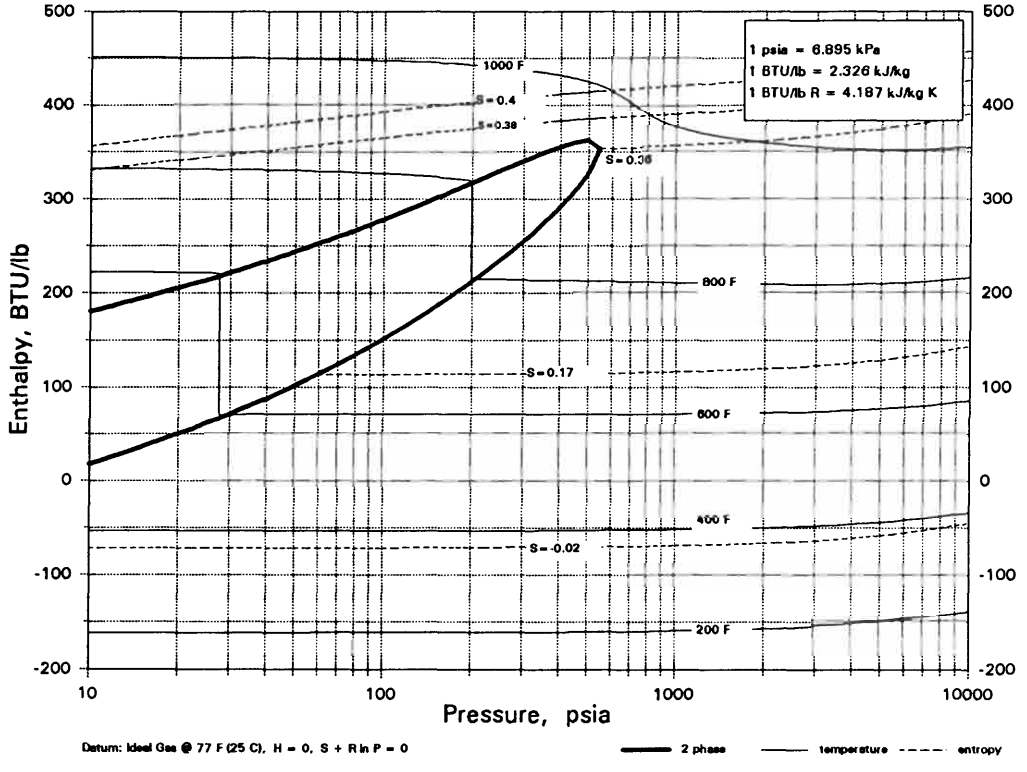
C10H14O p-tert-BUTYLPHENOL



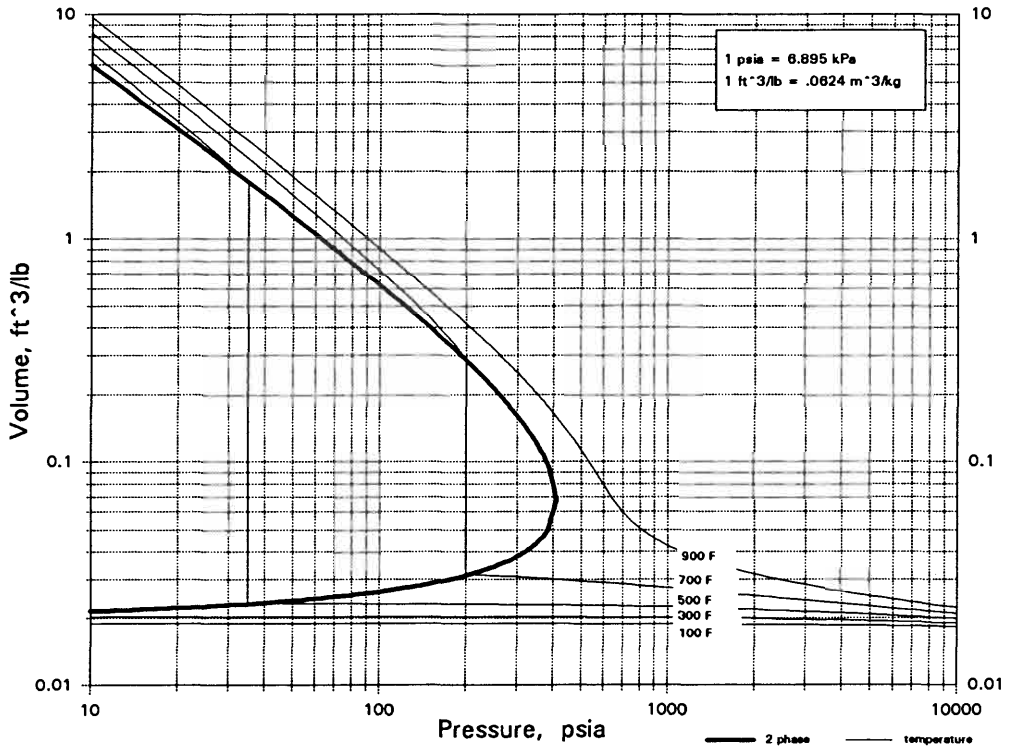


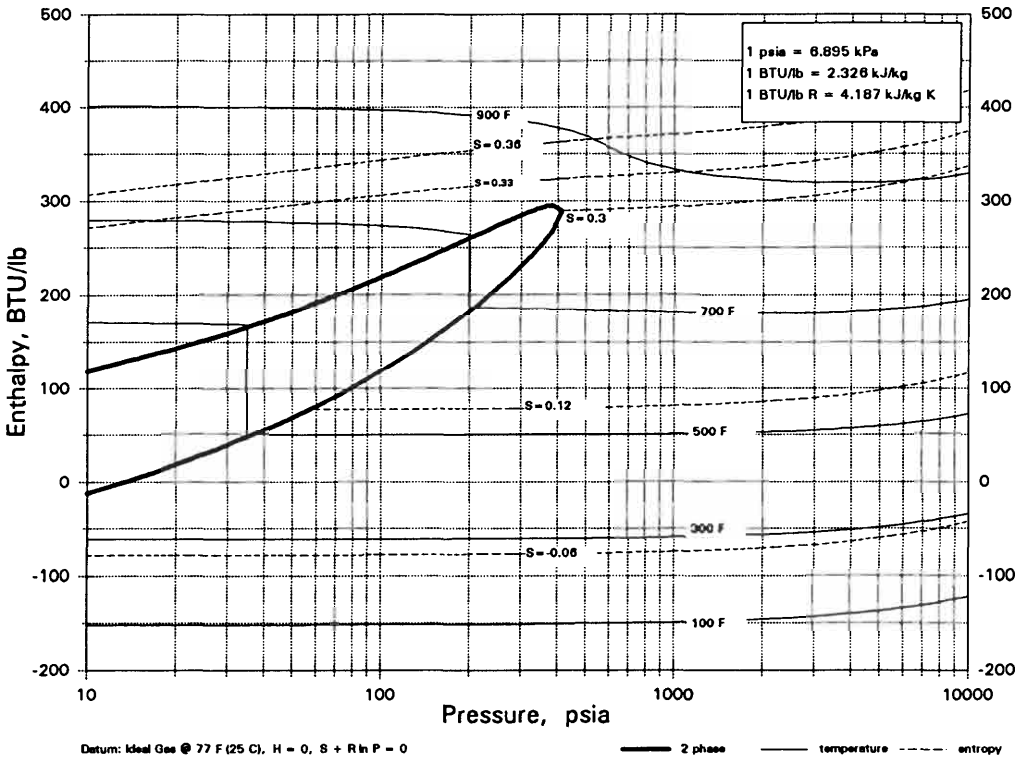
C10H14O2 p-tert-BUTYLCATECHOL



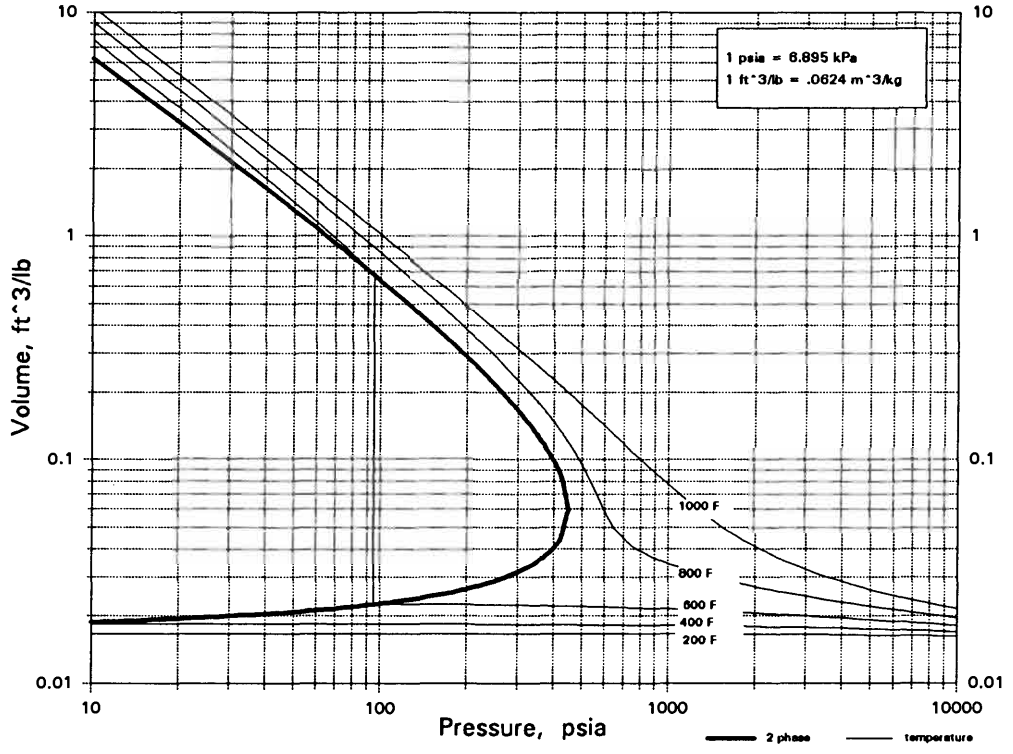


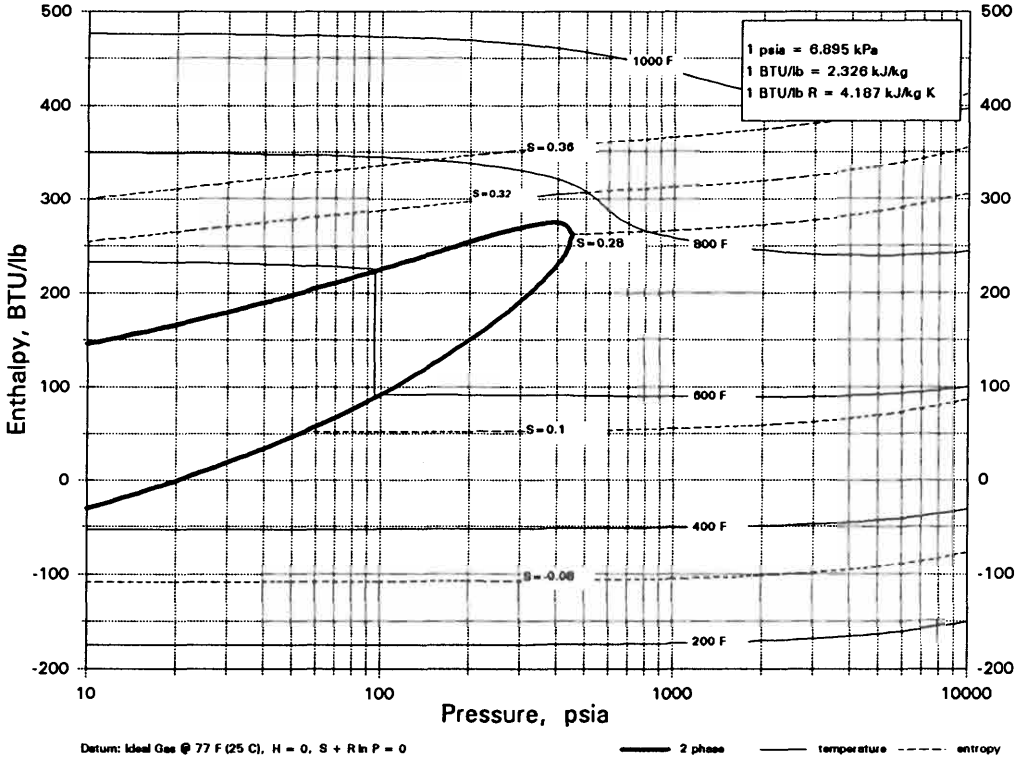
C10H15N N-N-DIETYHLANILINE



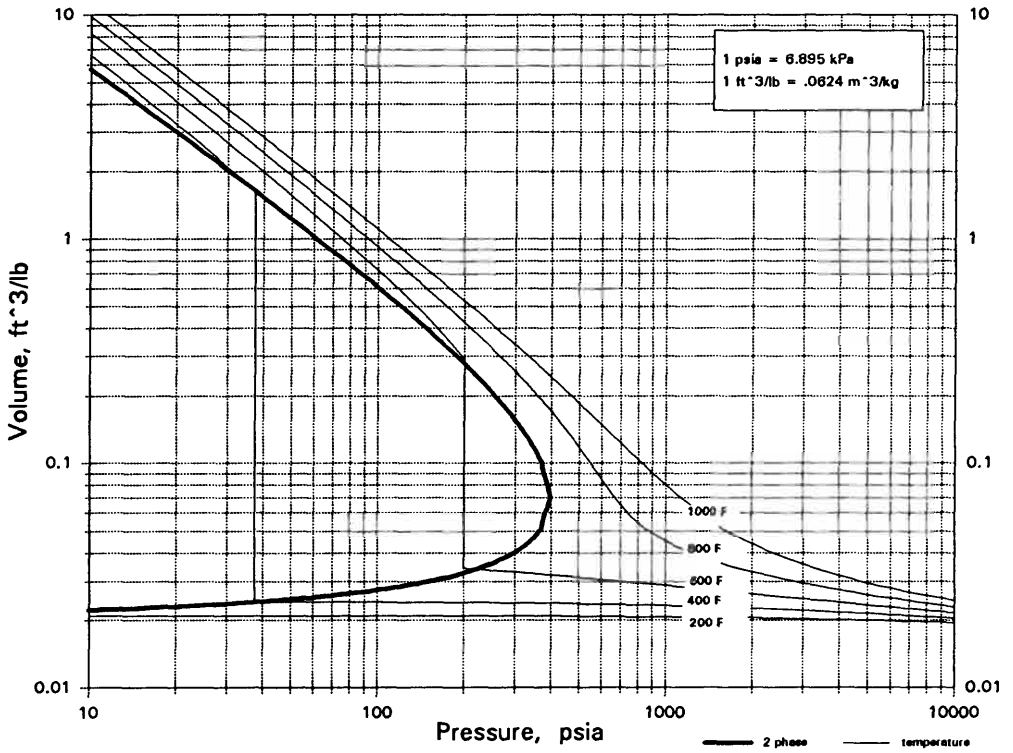


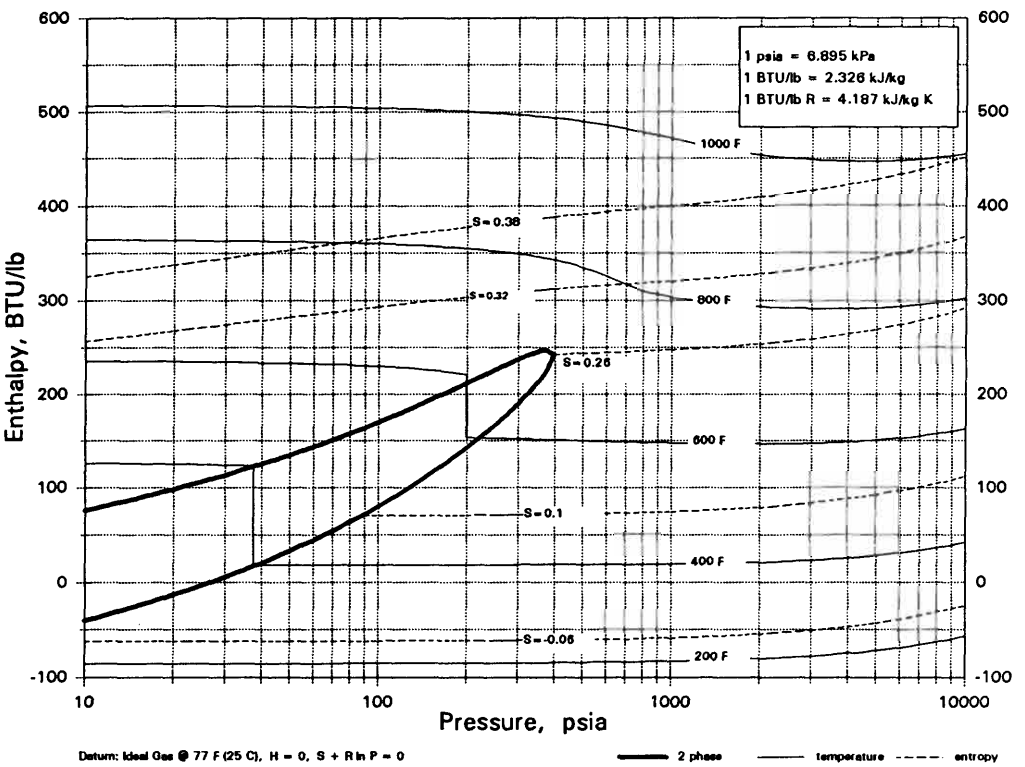
C10H15N 2-6-DIETHYLANILINE



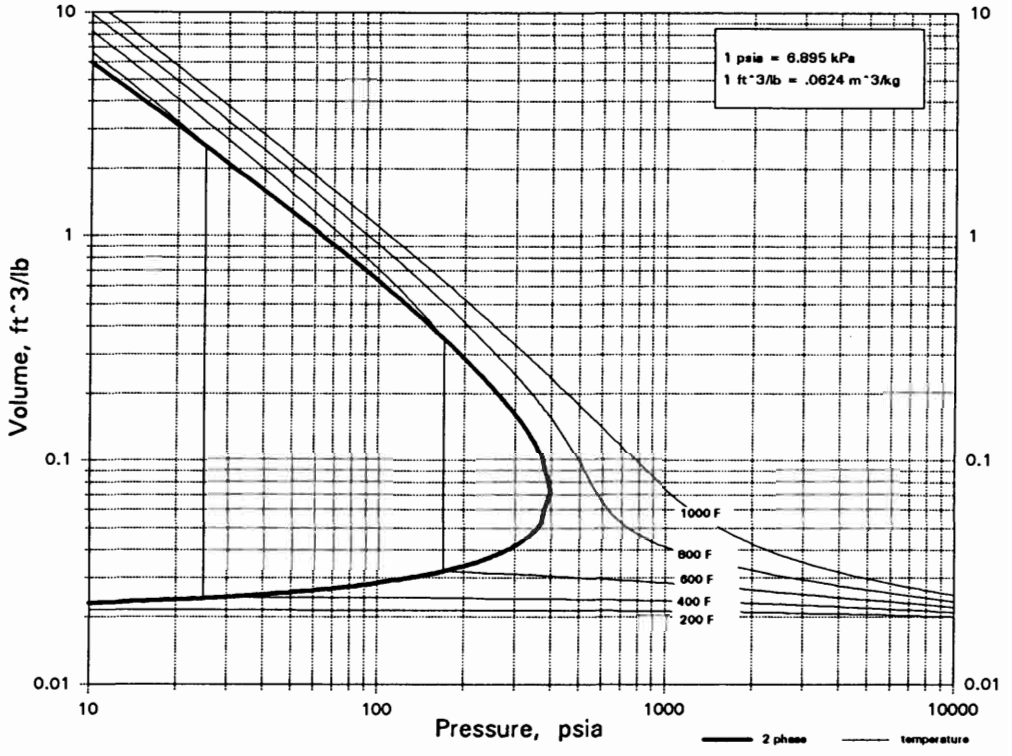


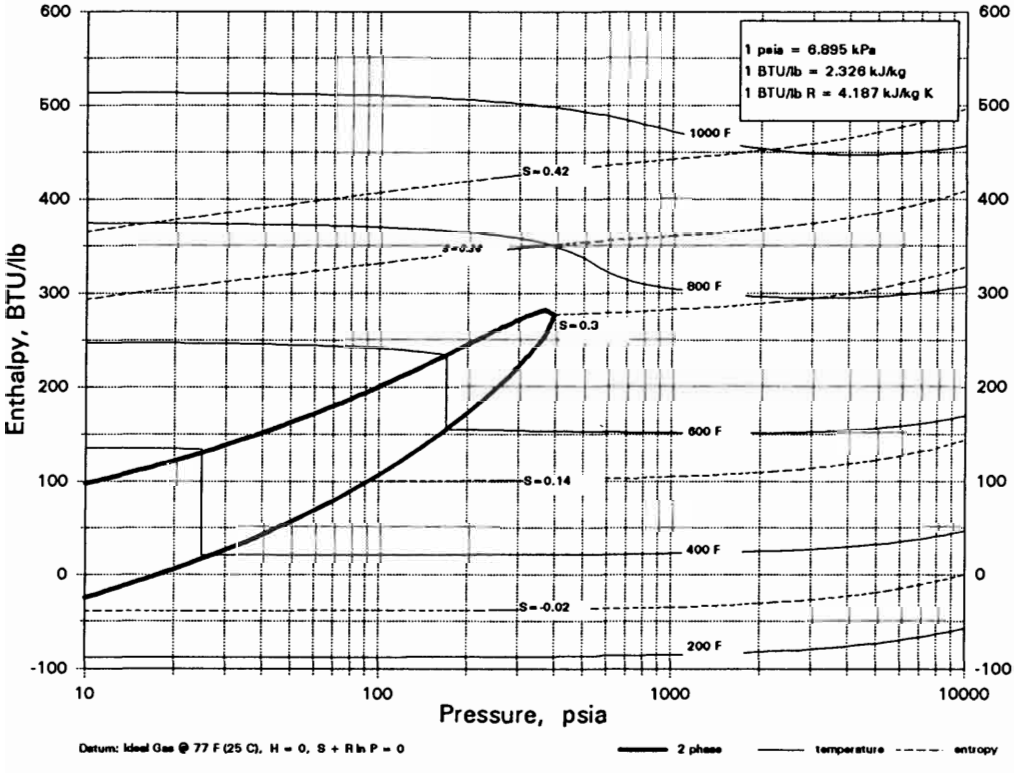
C10H16 CAMPHENE



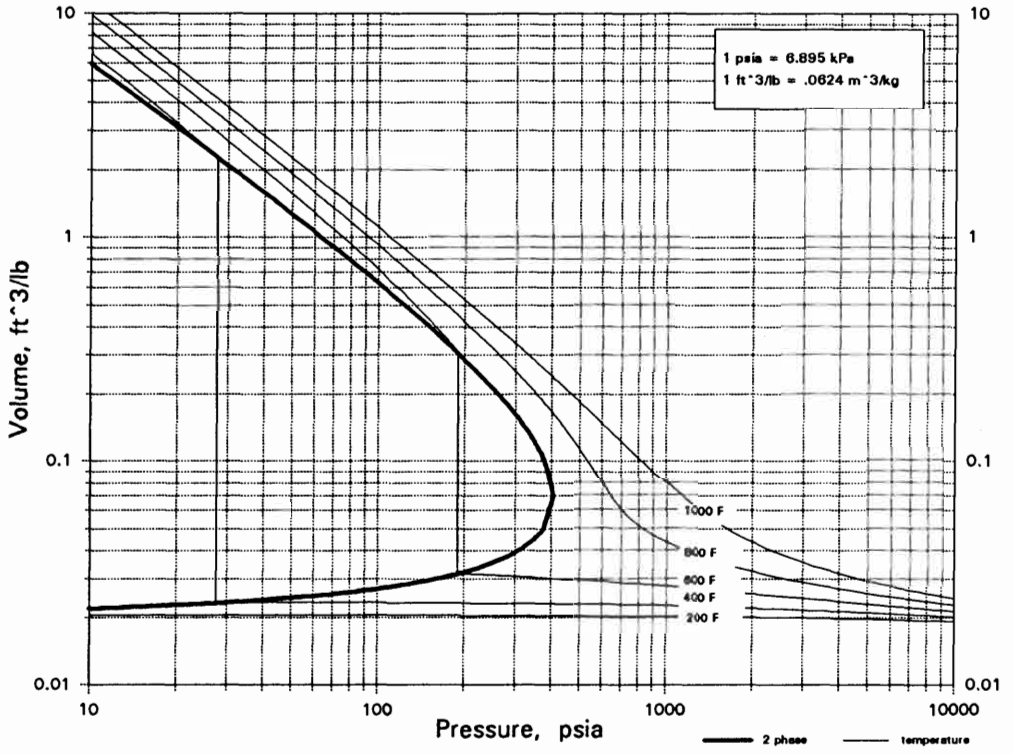


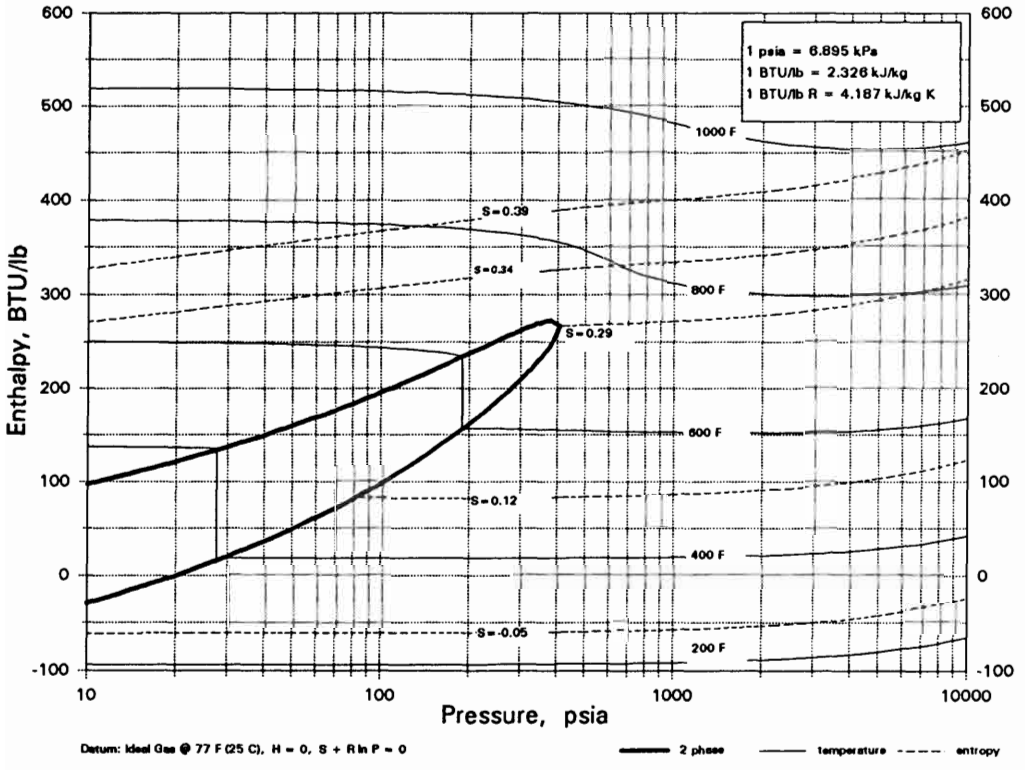
C10H16 D-LIMONENE



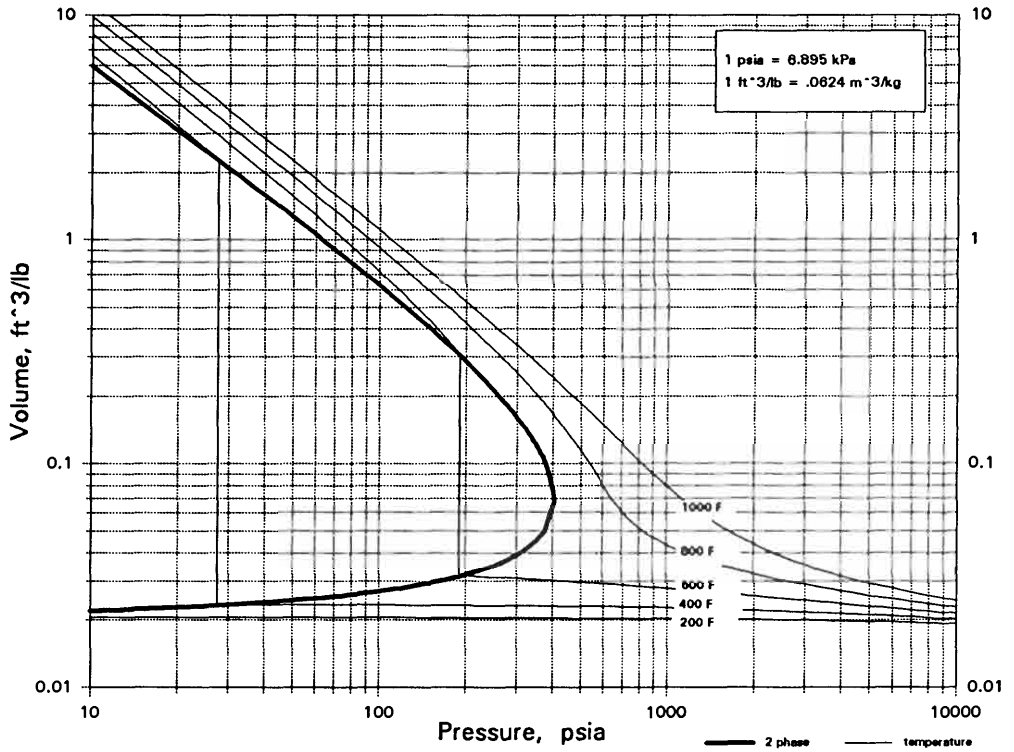


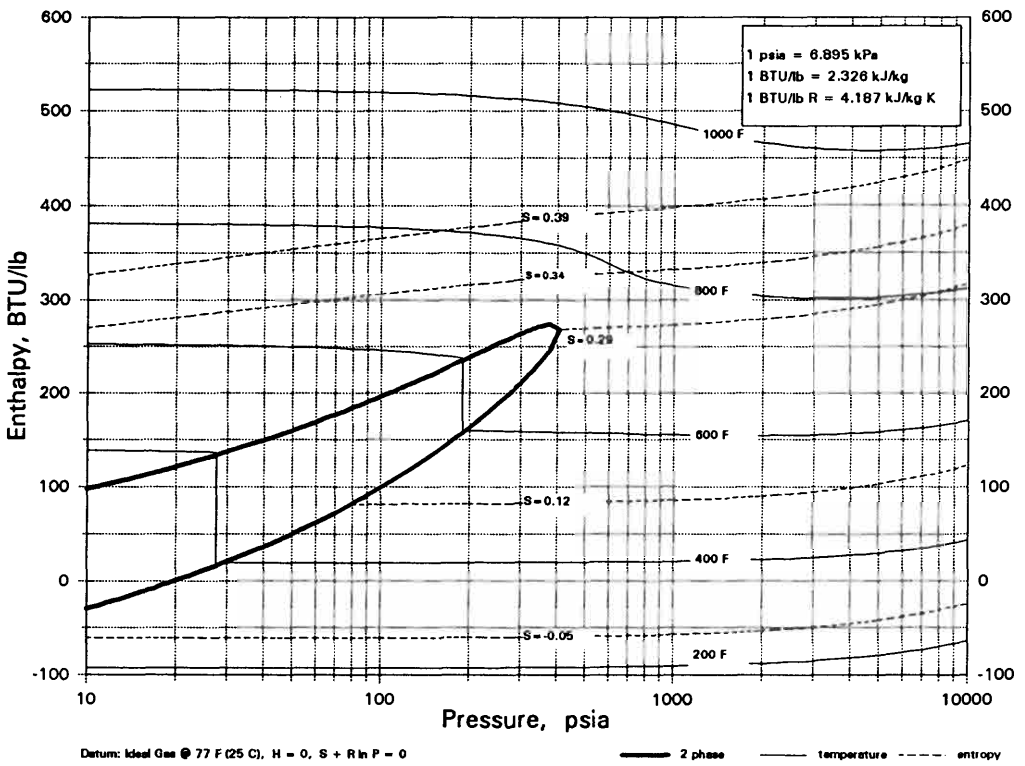
C10H16 alpha-PHELLANDRENE



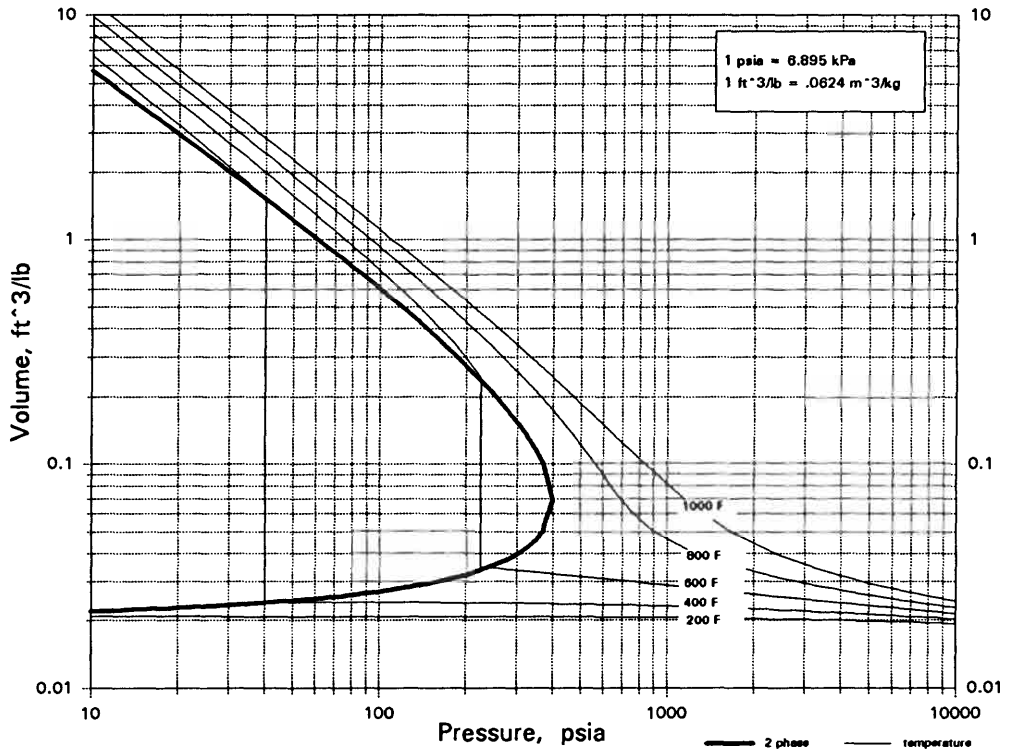


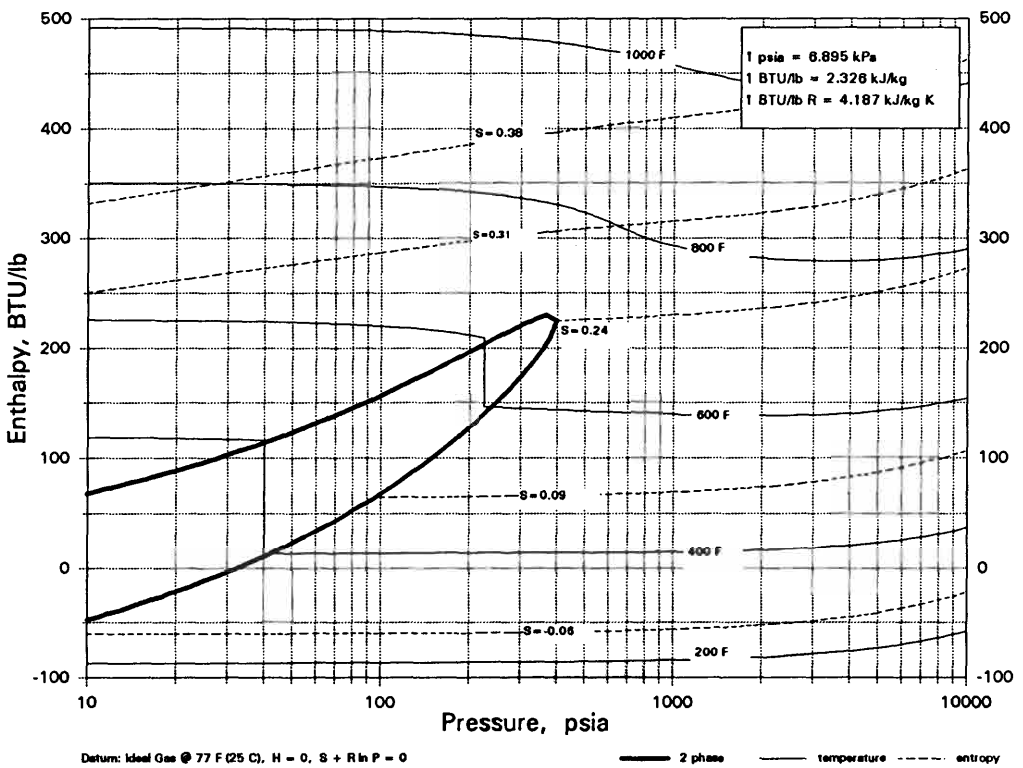
C1OH16 beta-PHELLANDRENE



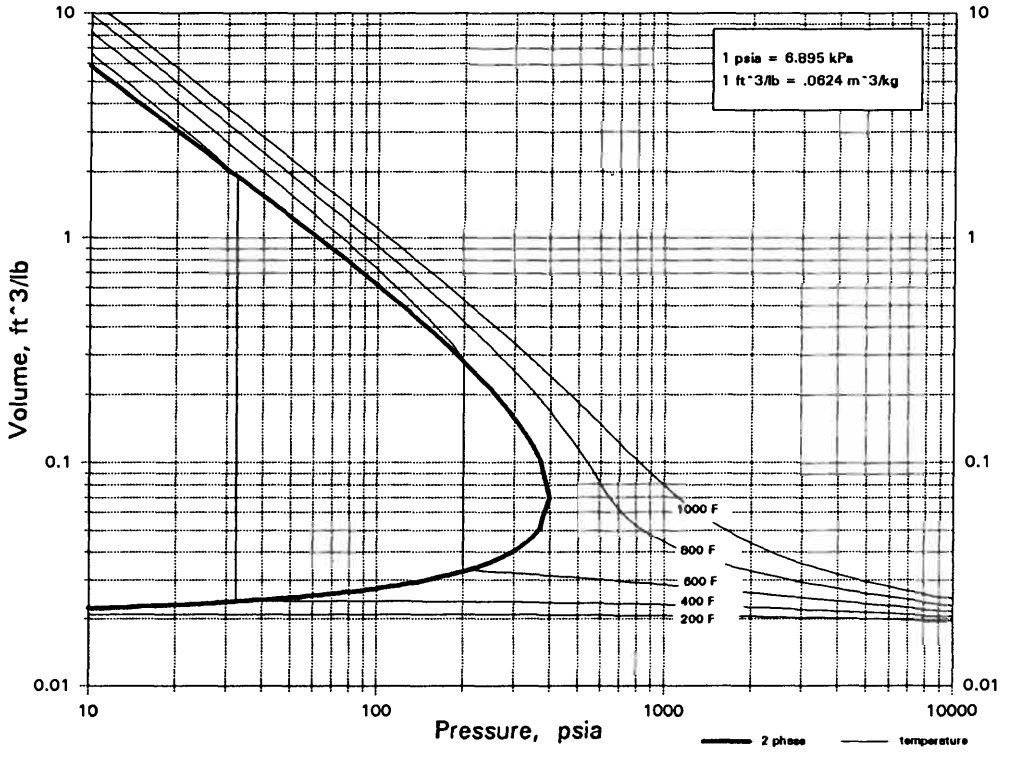


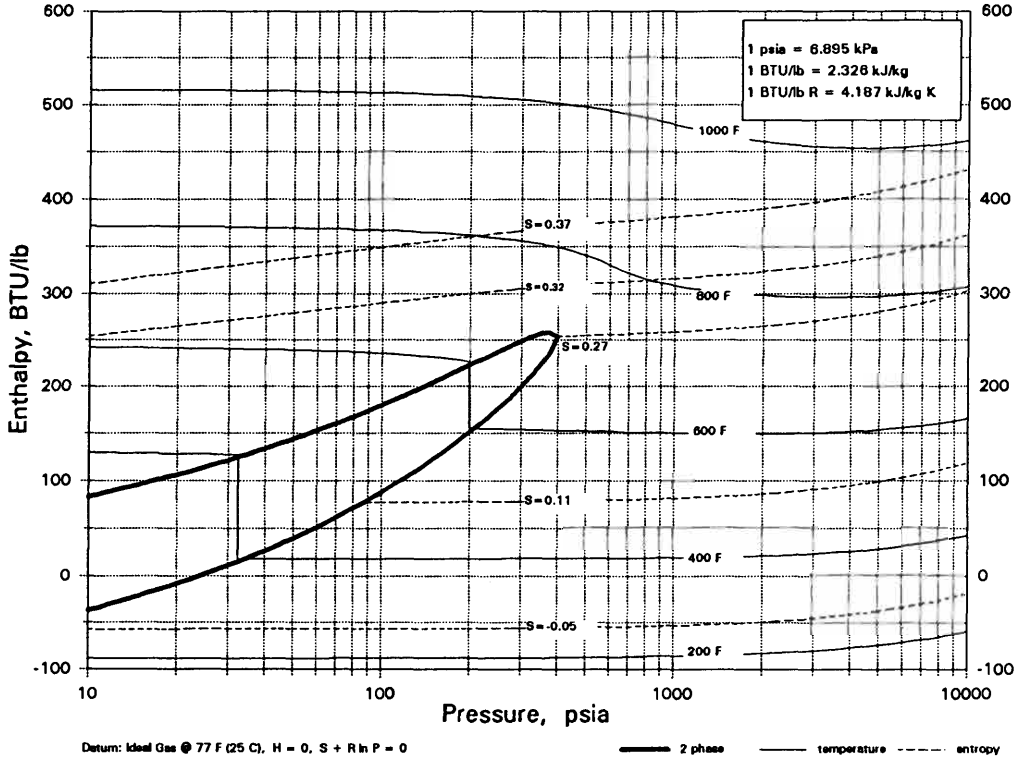
C10H16 alpha-PINENE



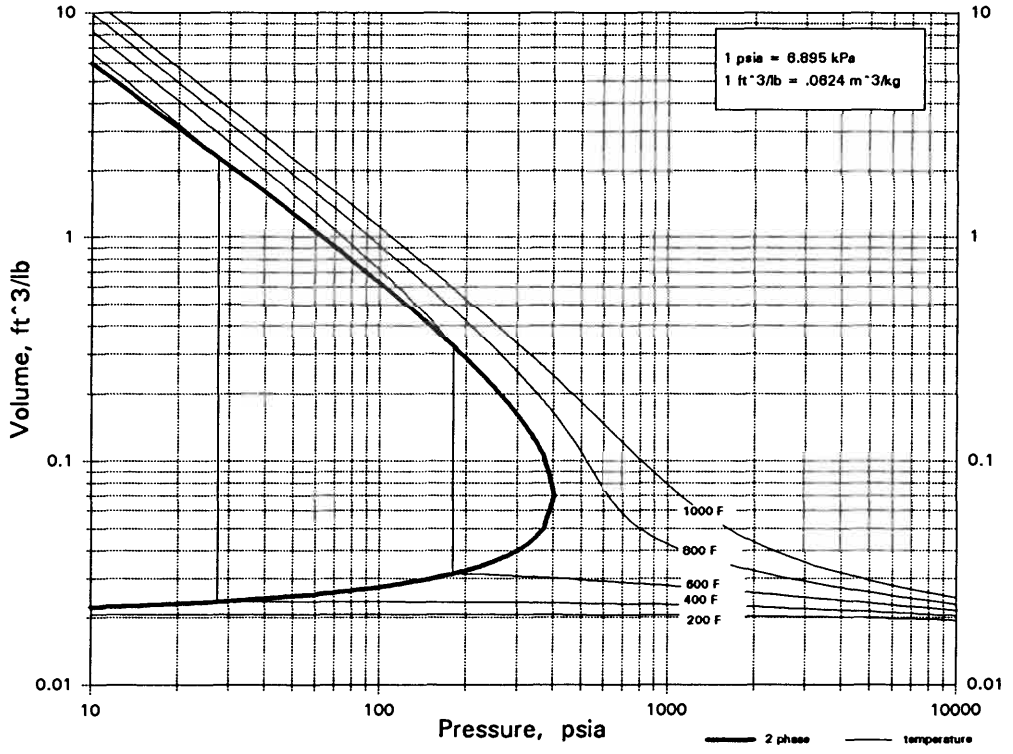


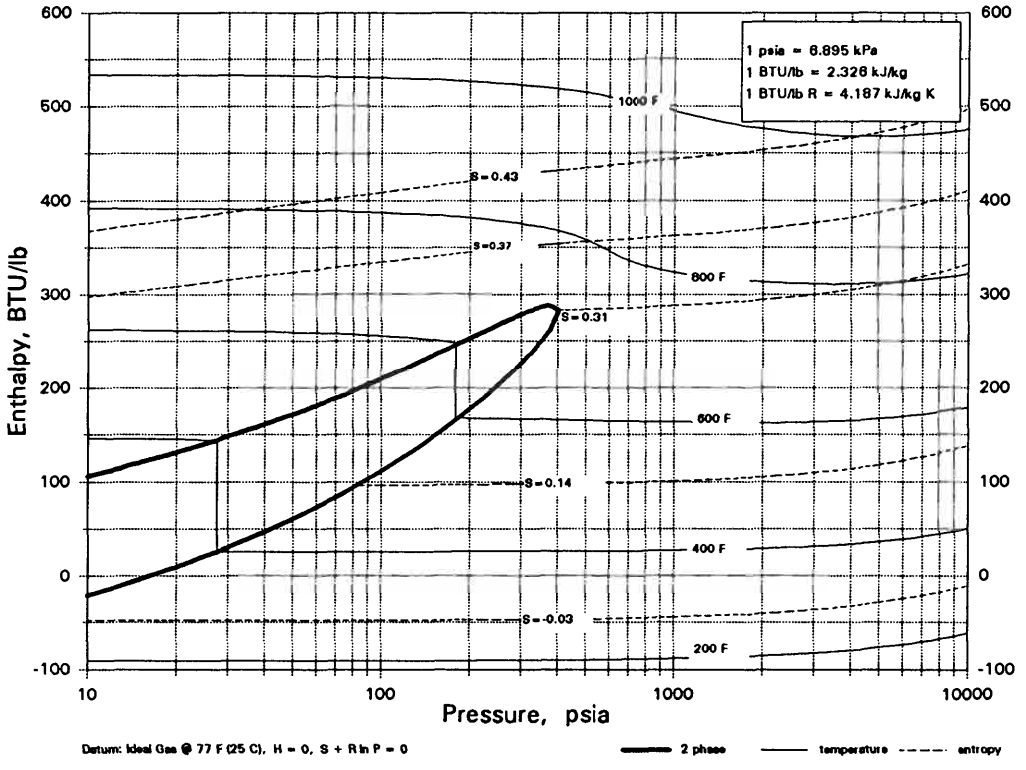
C10H16 beta-PINENE



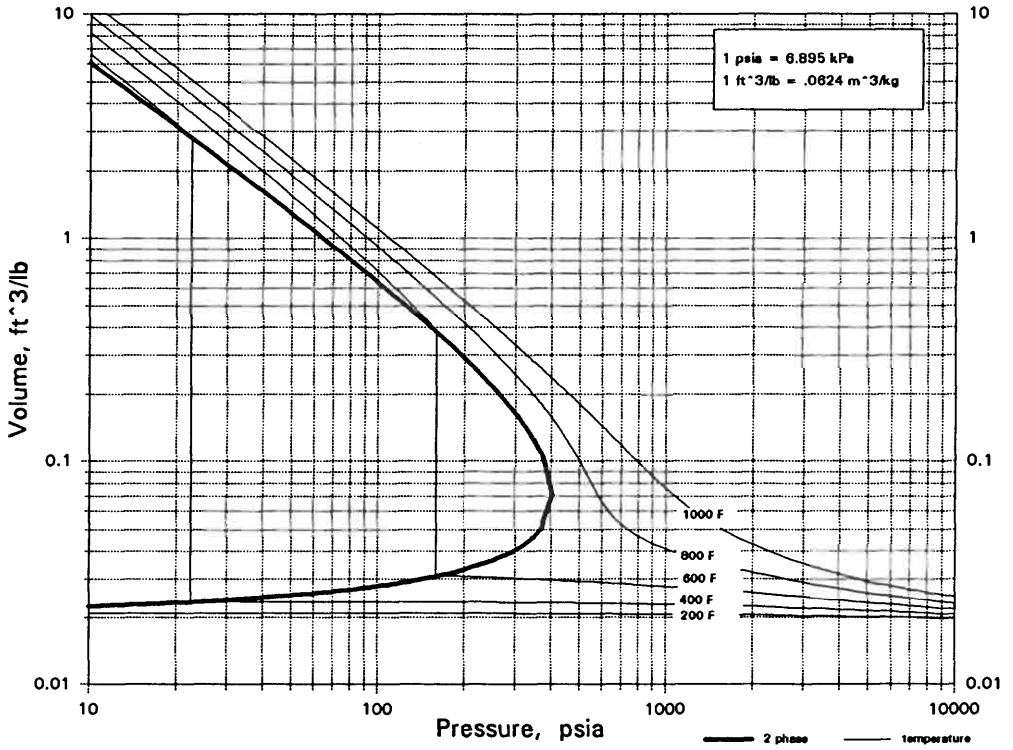


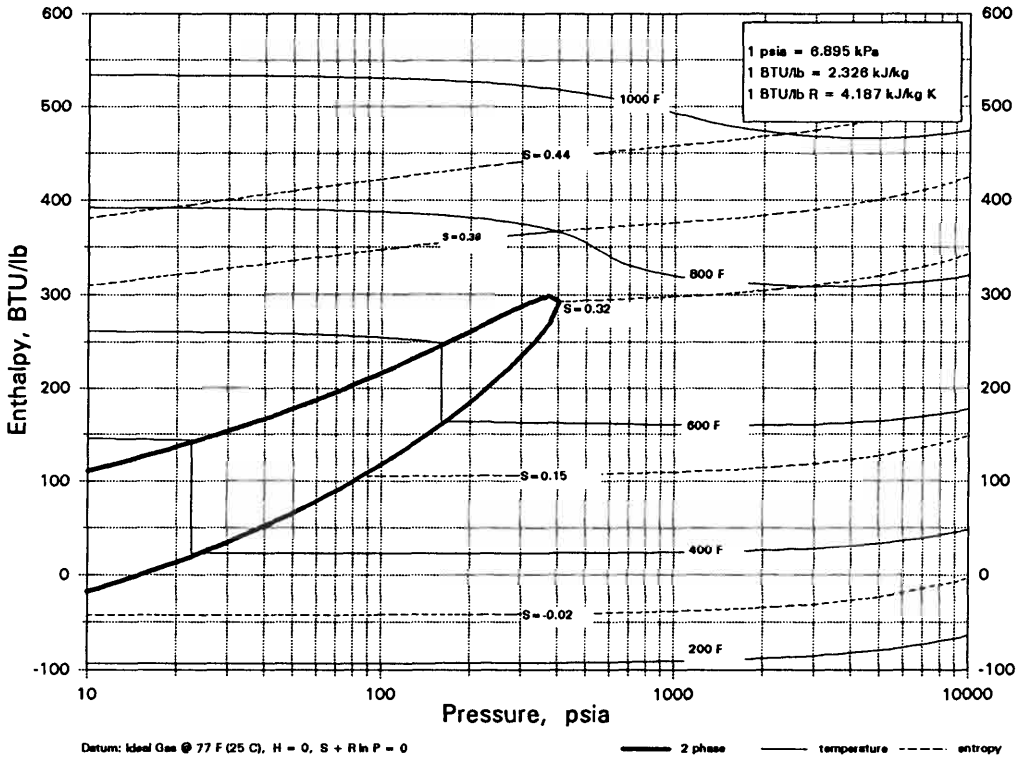
C10H16 alpha-TERPINENE



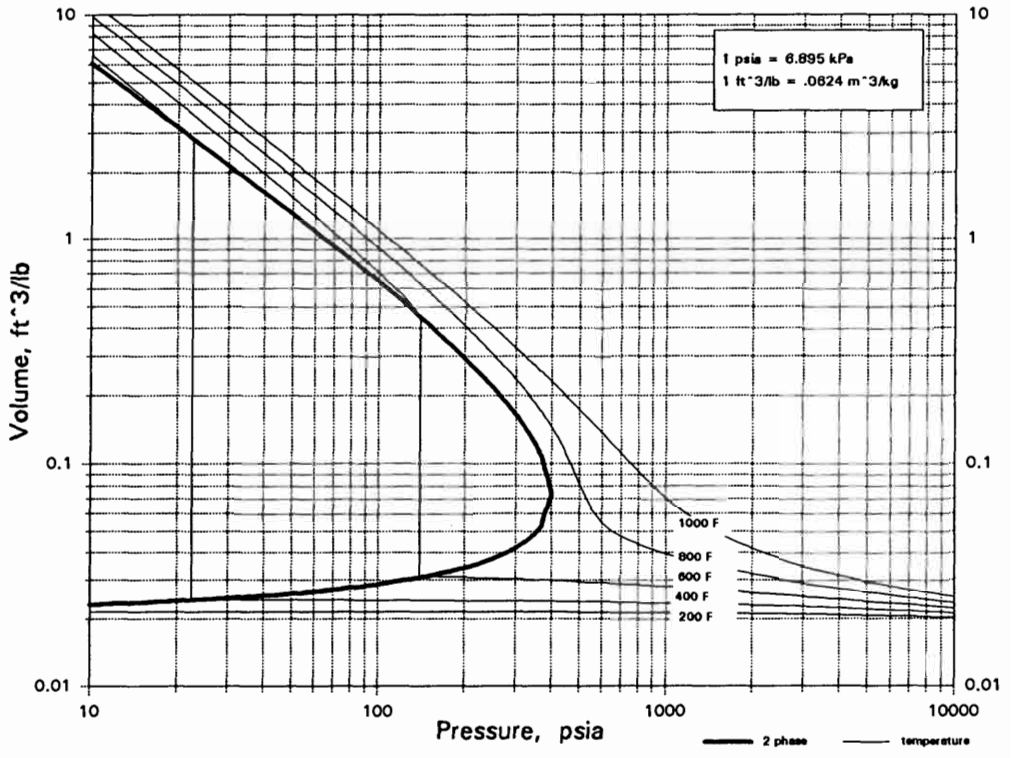


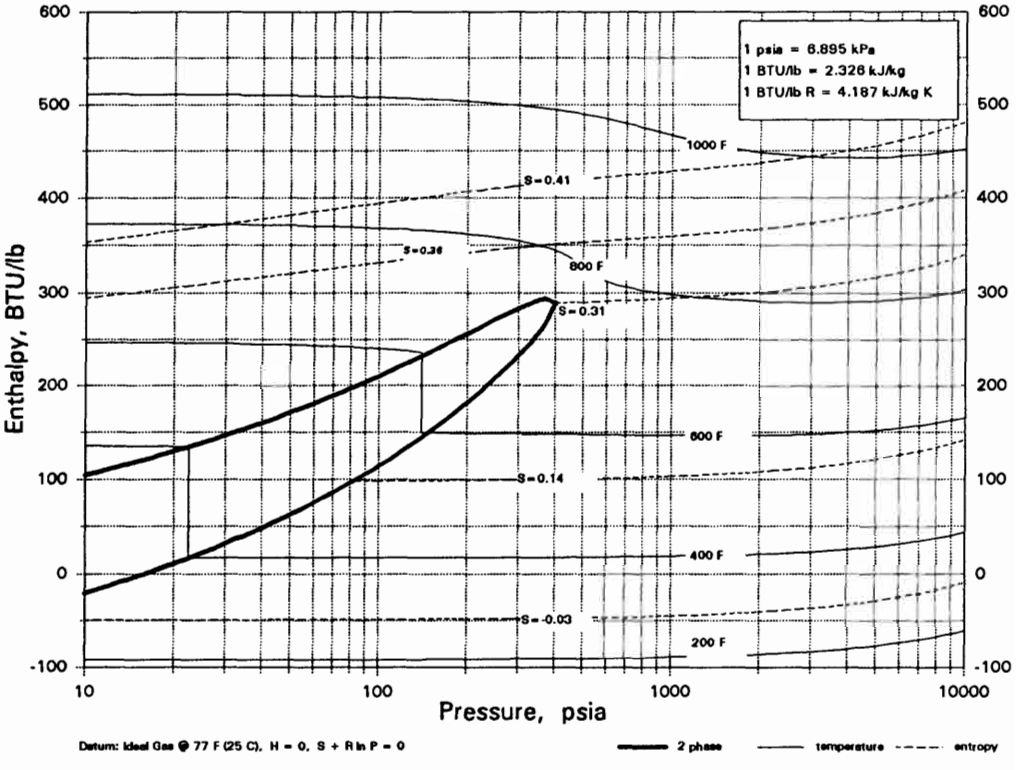
C1OH16 gamma-TERPINENE



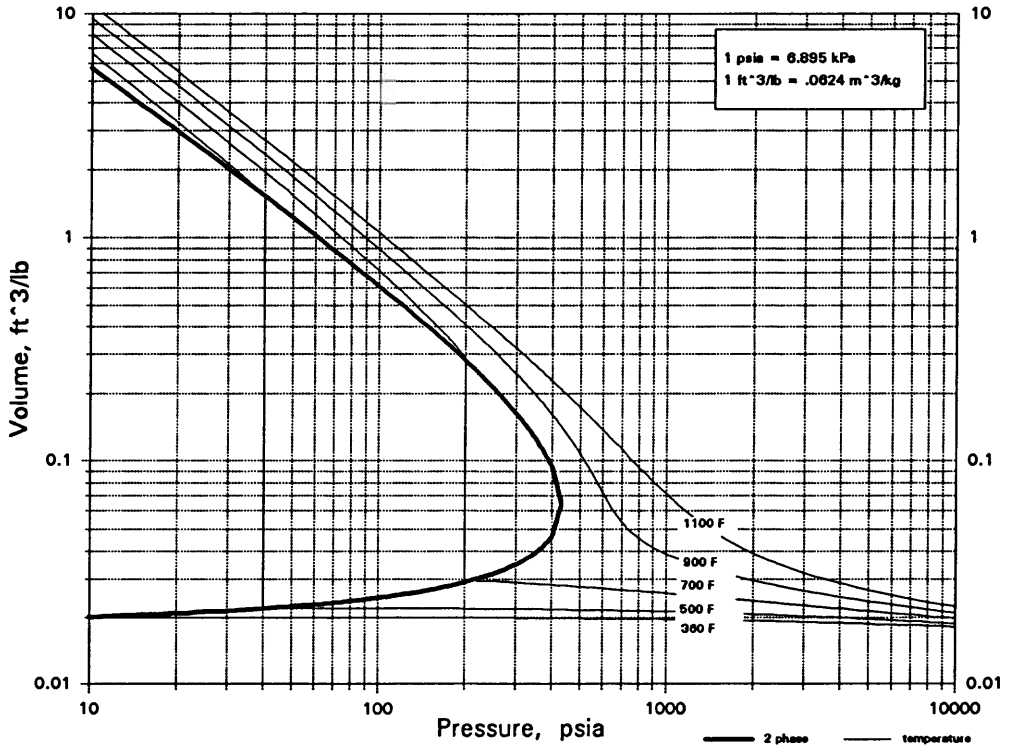


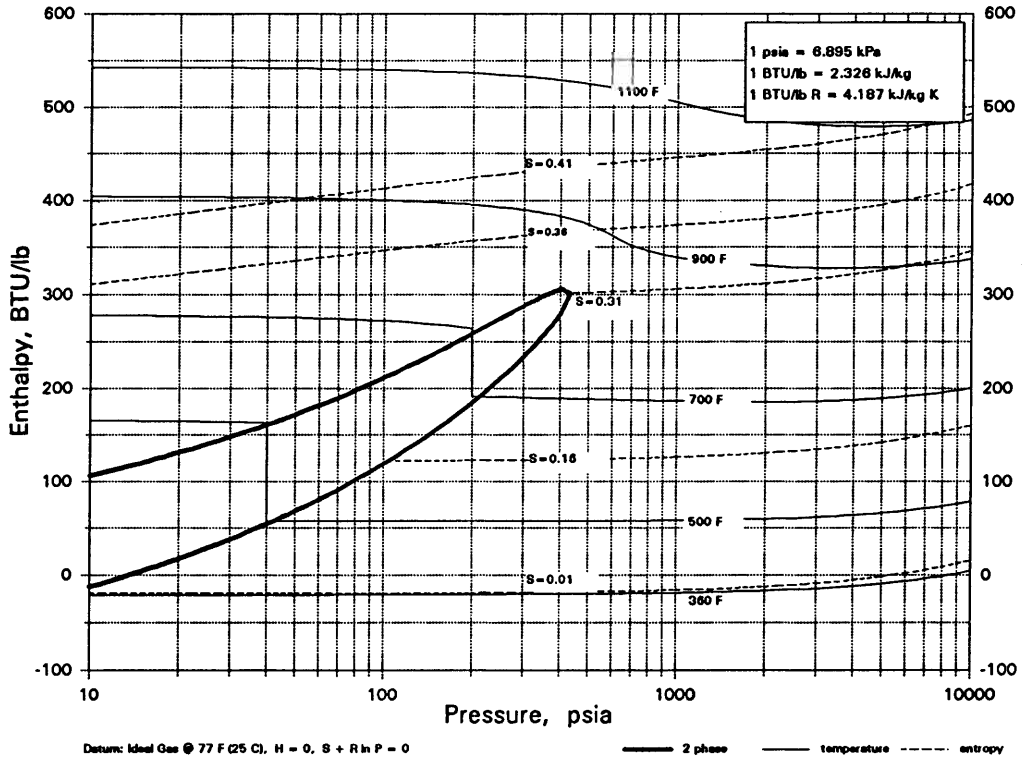
C10H16 TERPINOLENE



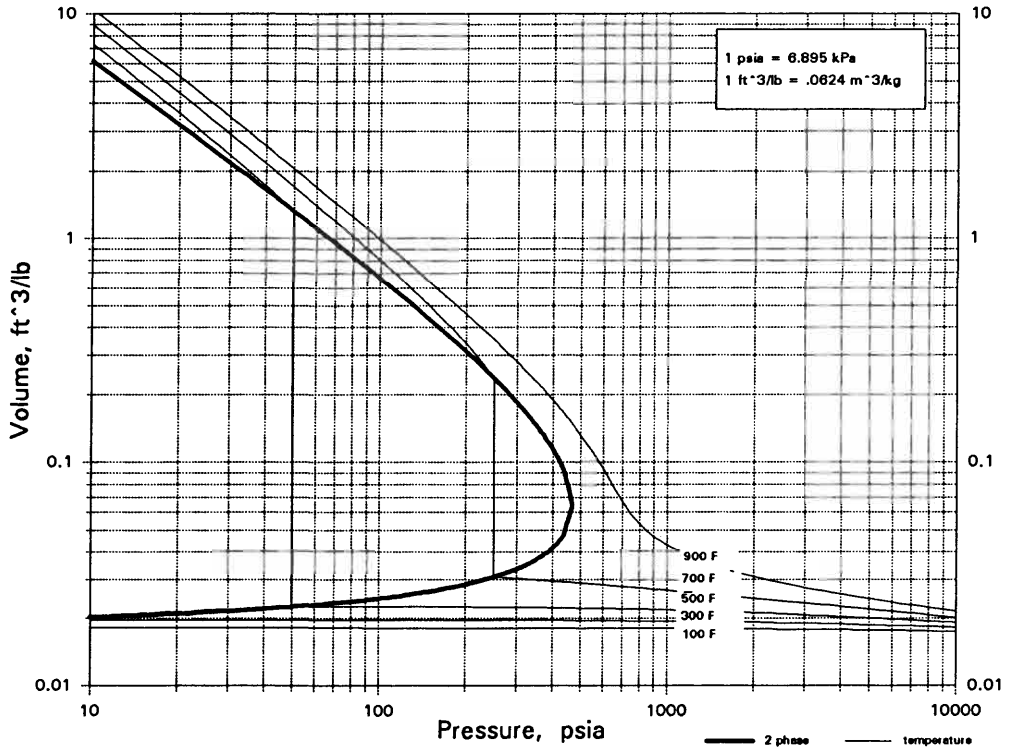


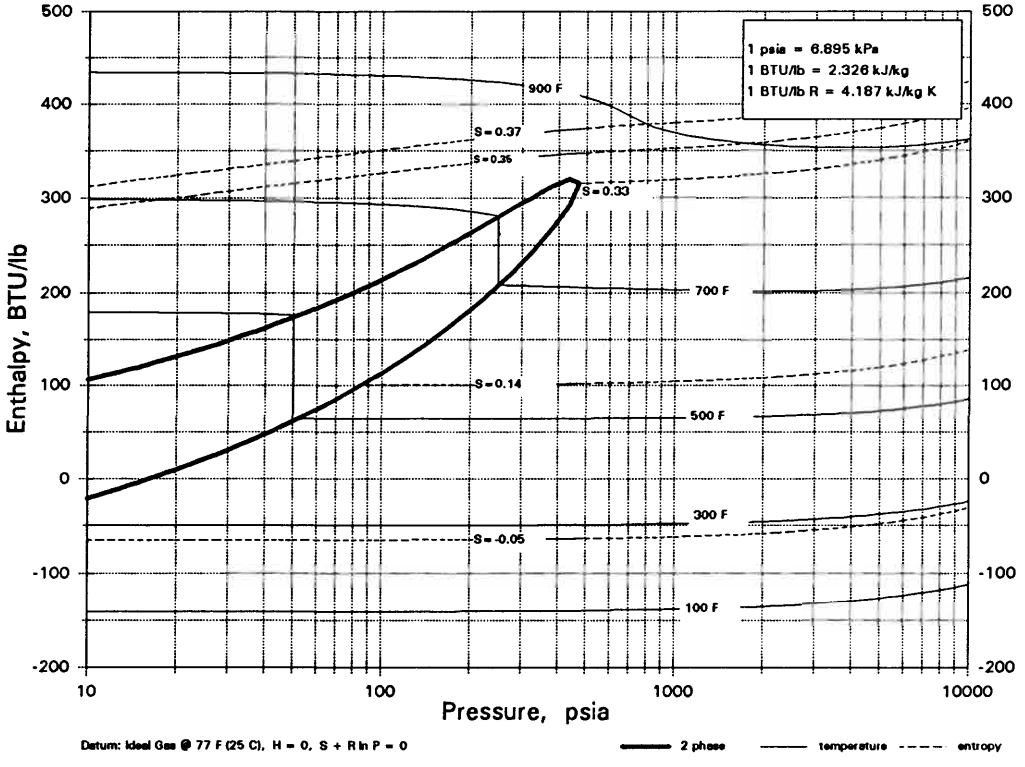
C10H16O CAMPHOR



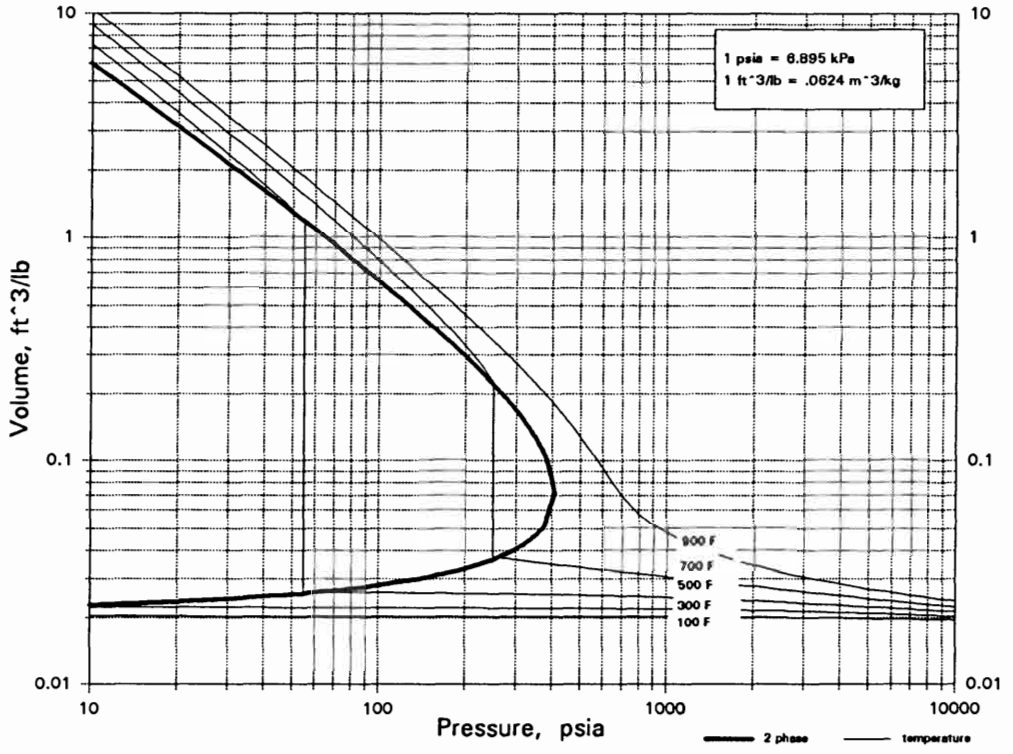


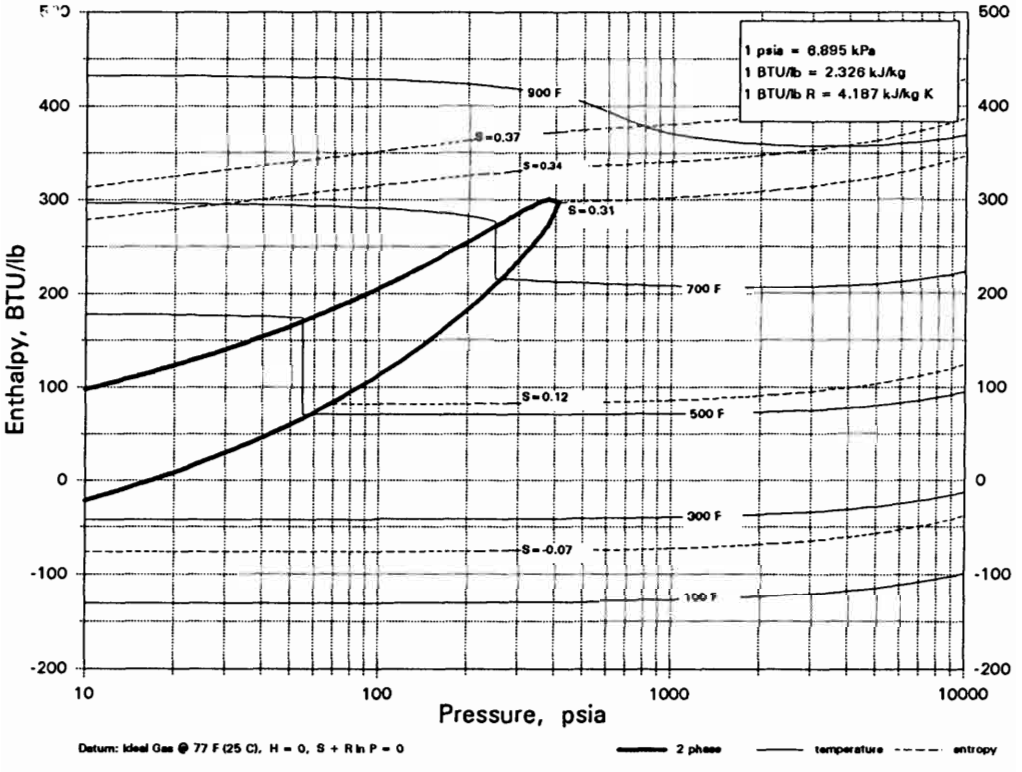
C10H18	cis-DECAHYDRONANPHTALENE



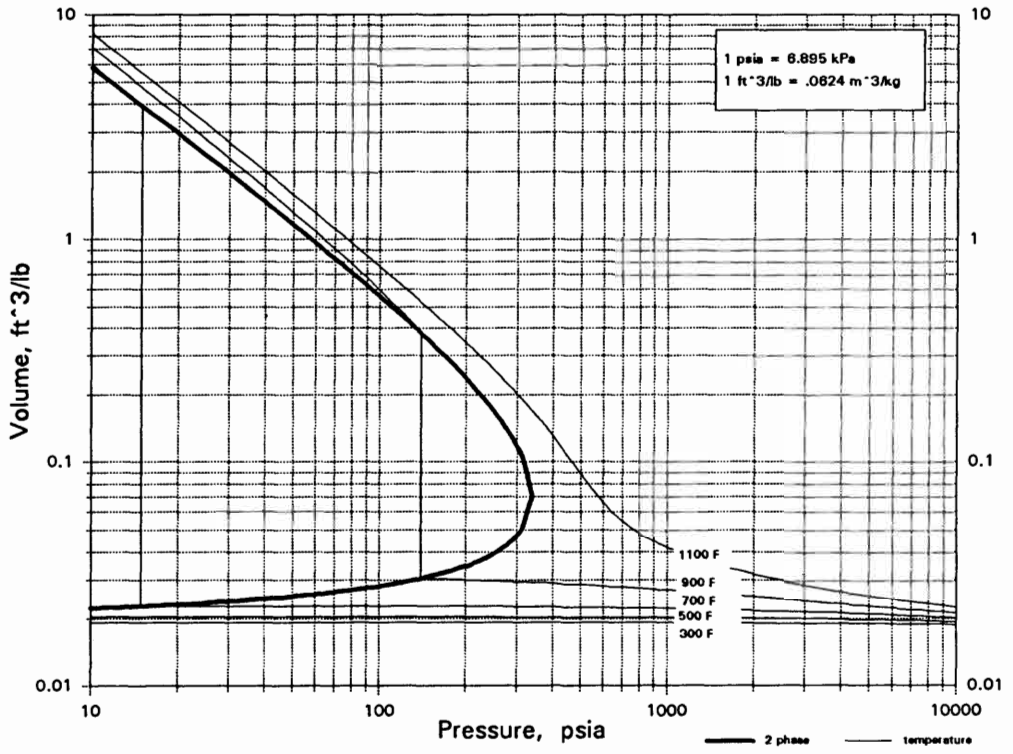


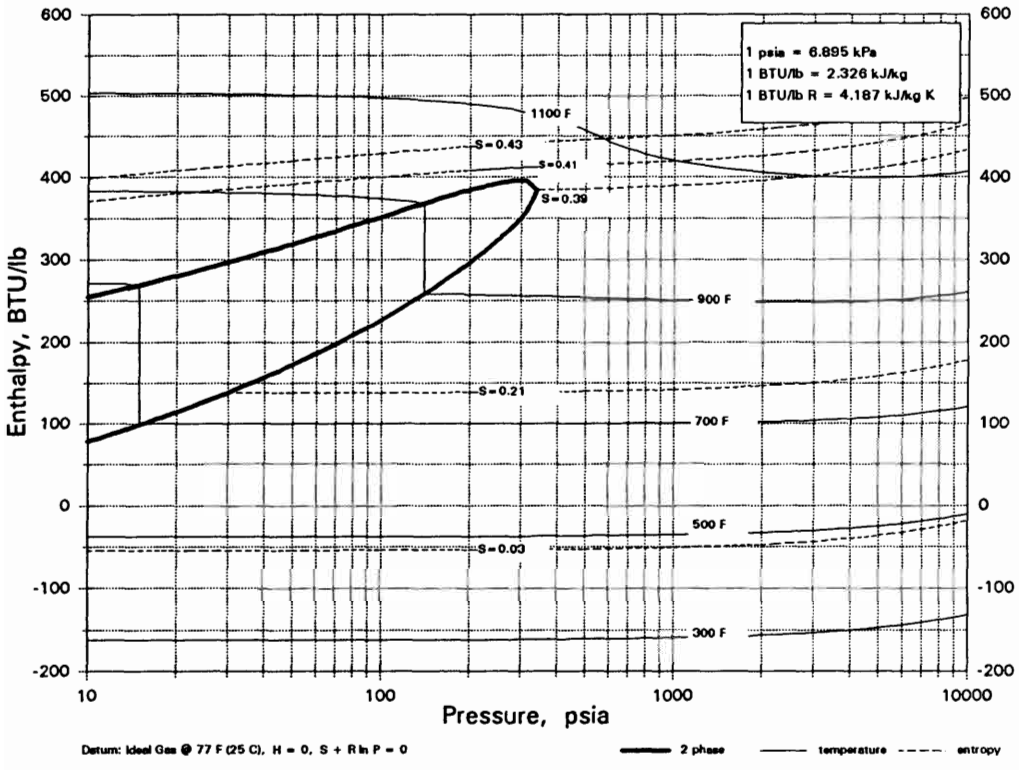
C10H18 trans-DECAHYDRONAPHTHALENE



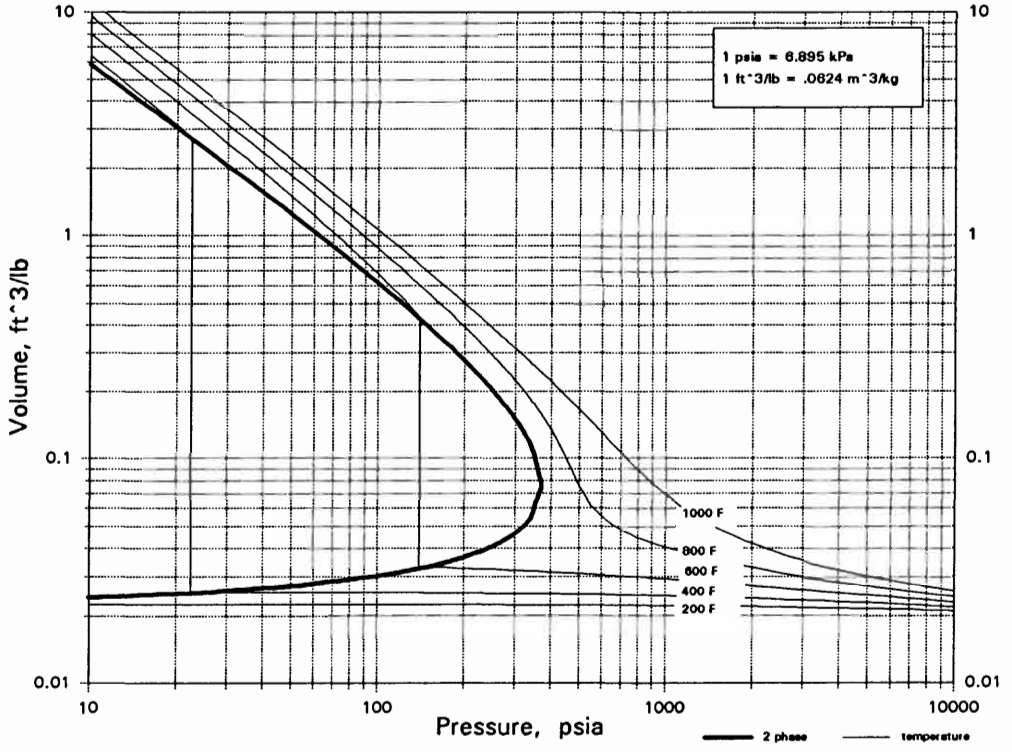


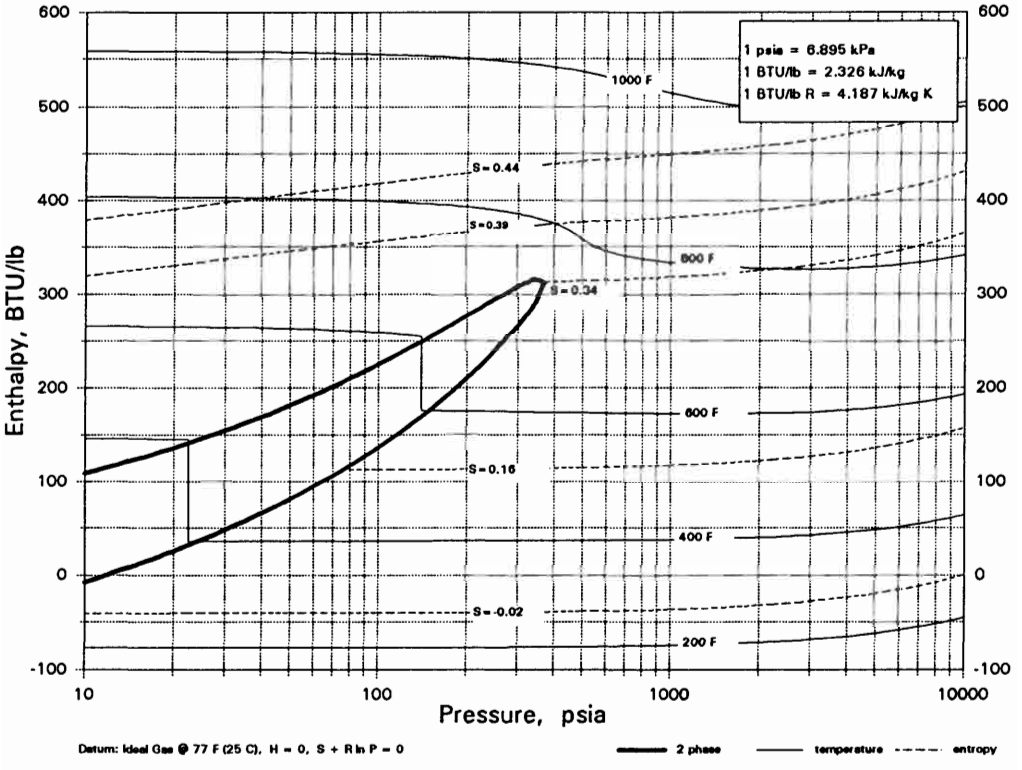
C10H18O4 SEBACIC ACID



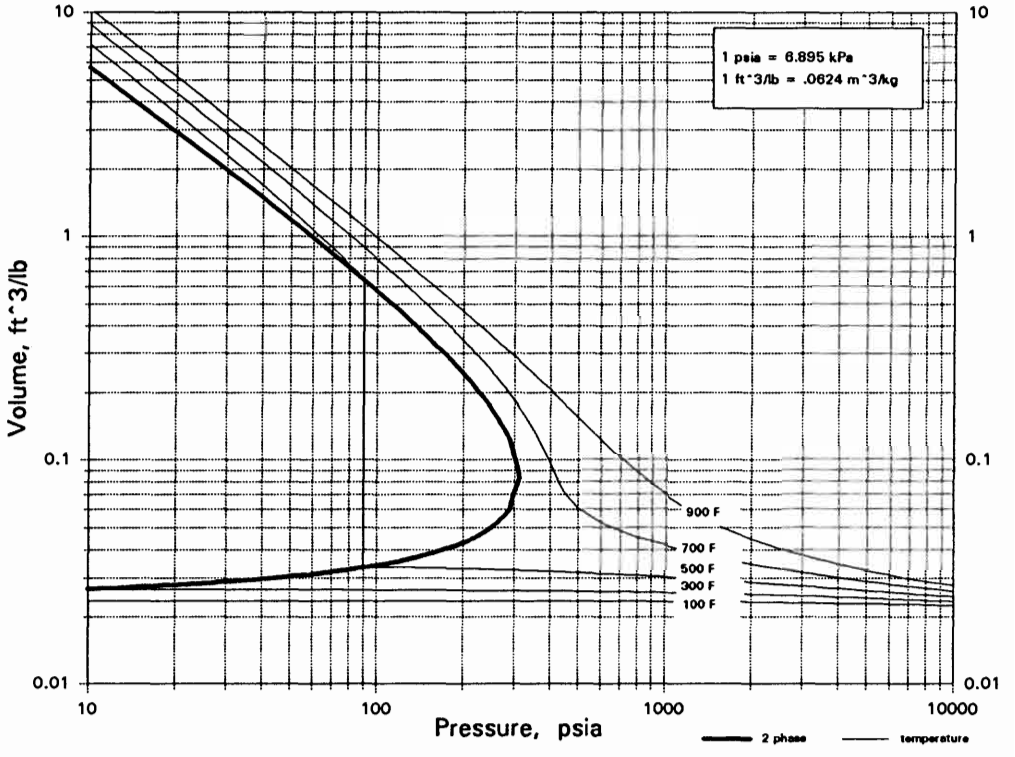


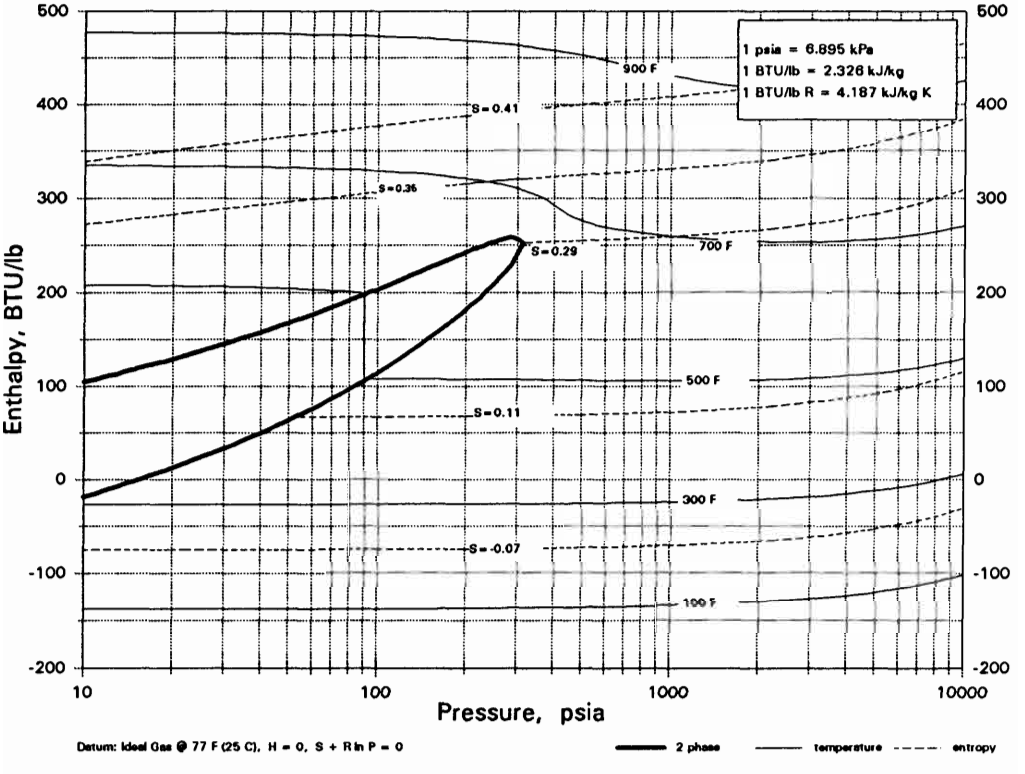
C10H20 n-BUTYLCYCLOHEXANE



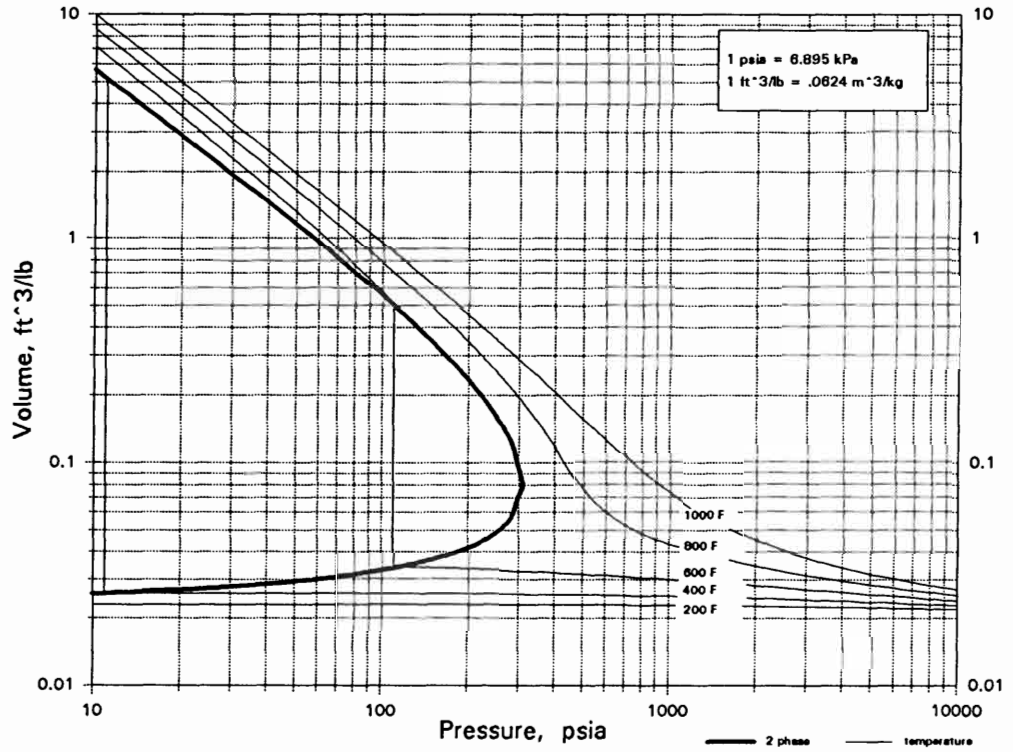


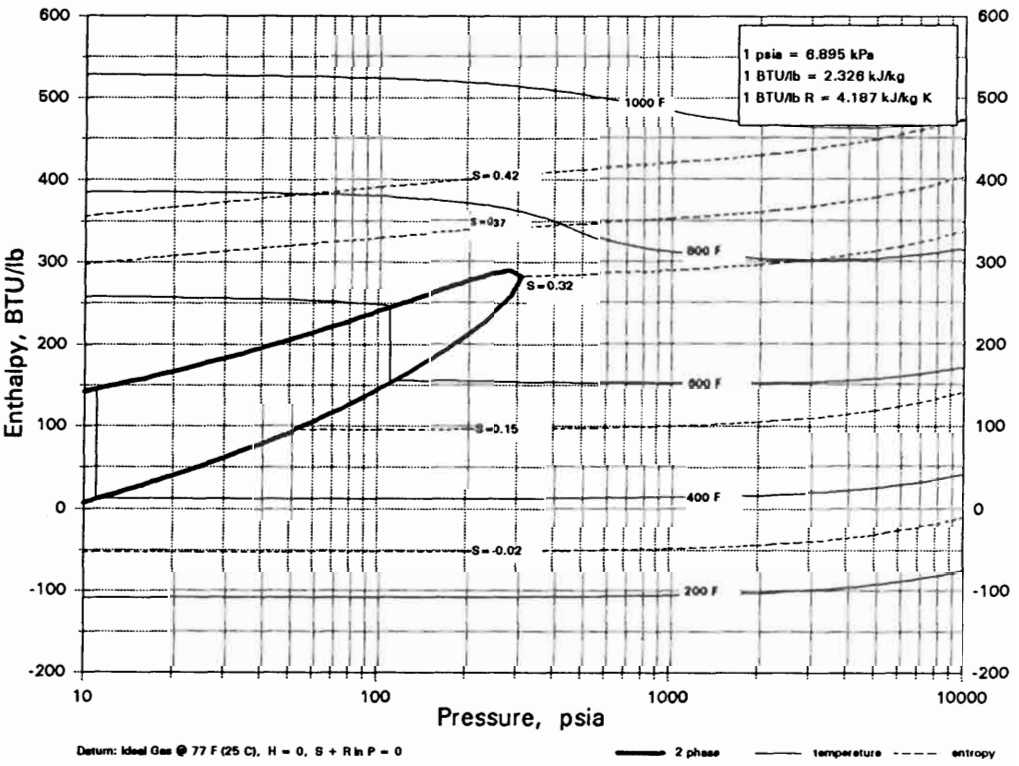
C10H20 1-DECENE



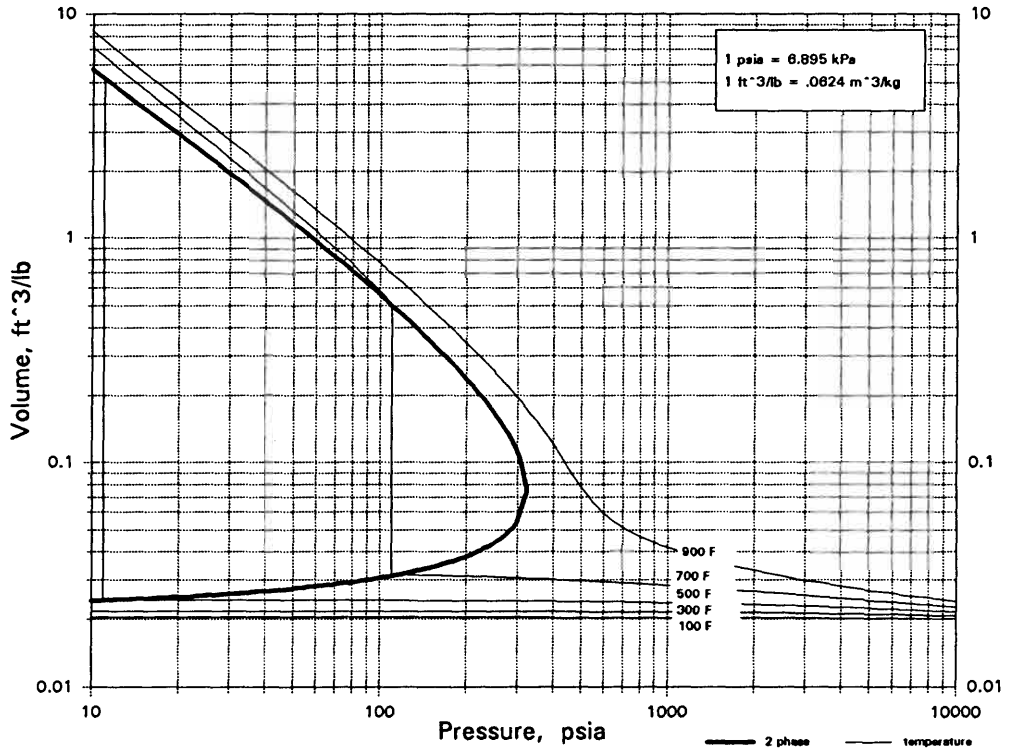


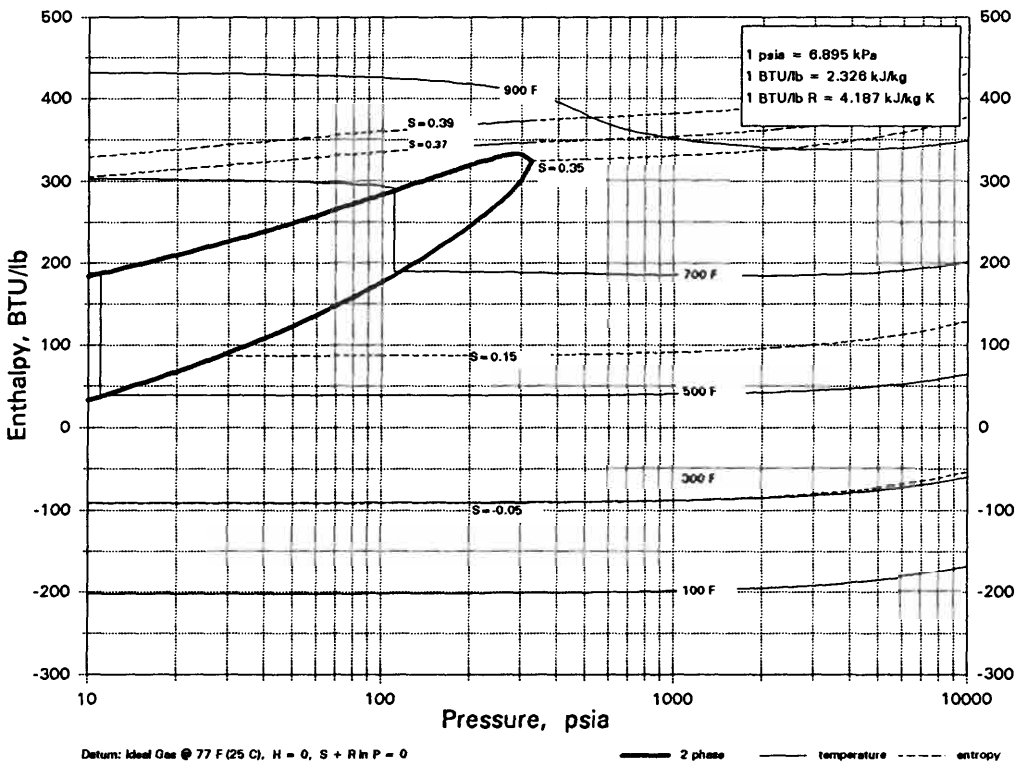
C10H20O 1-DECANAL



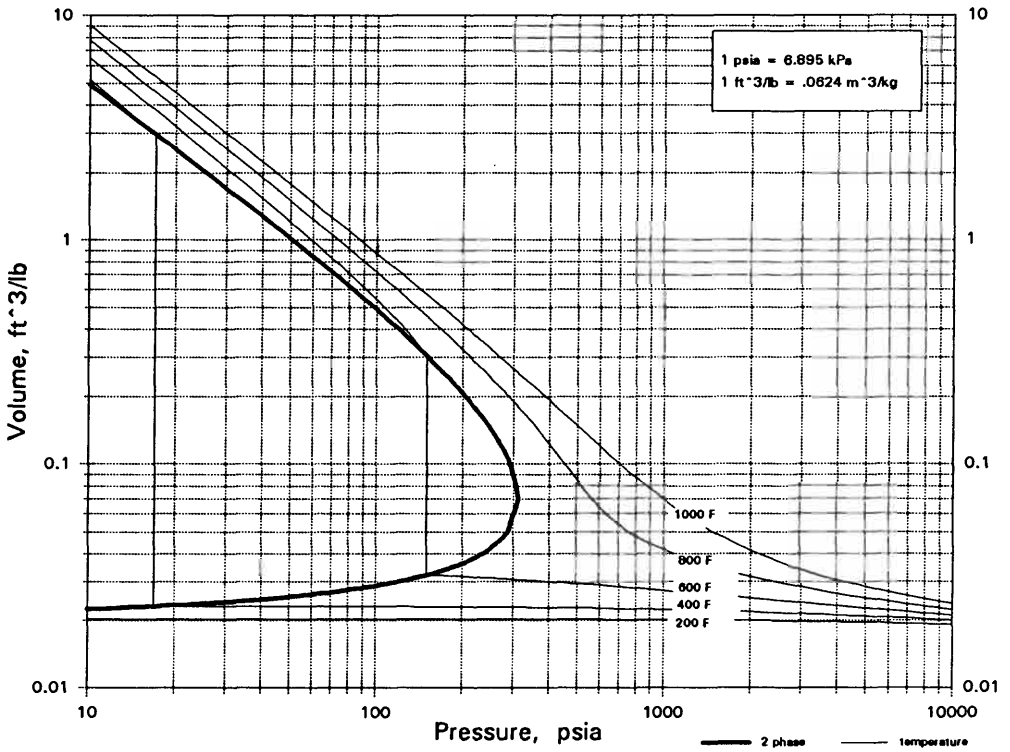


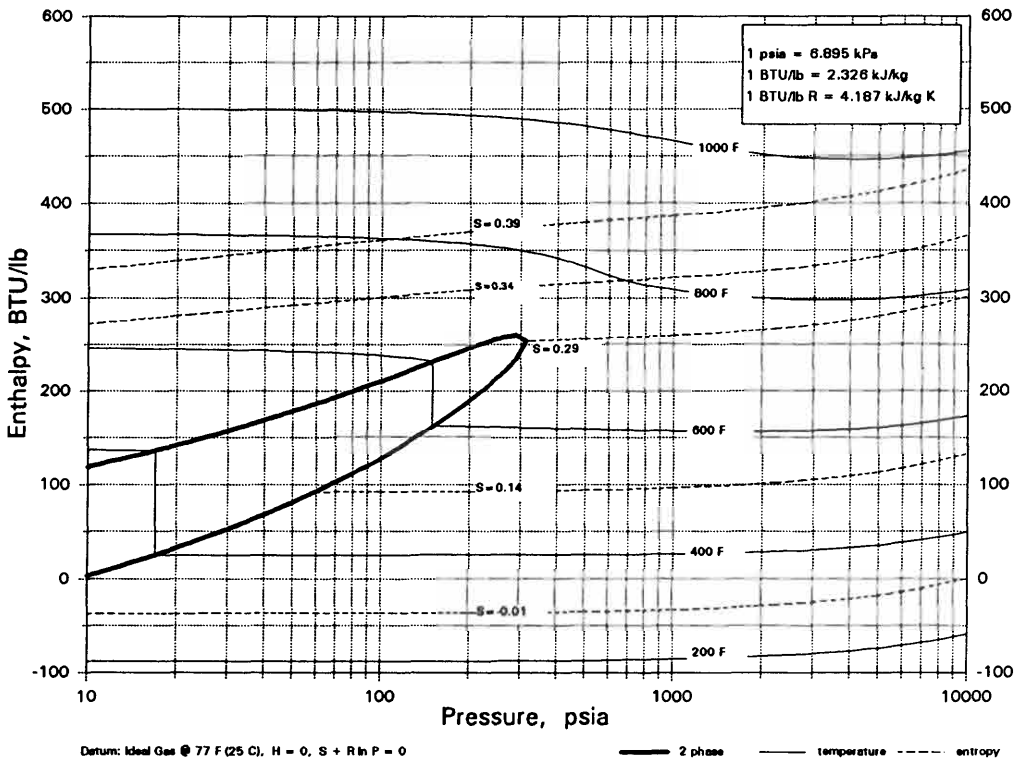
C10H20O2 n-DECANOIC ACID



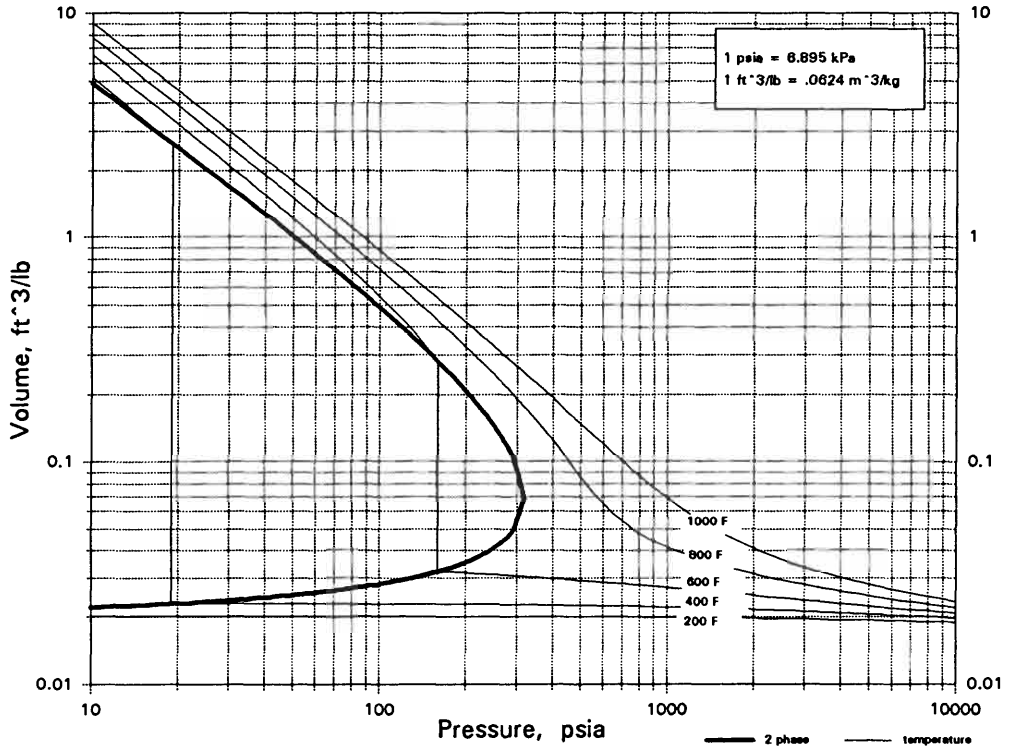


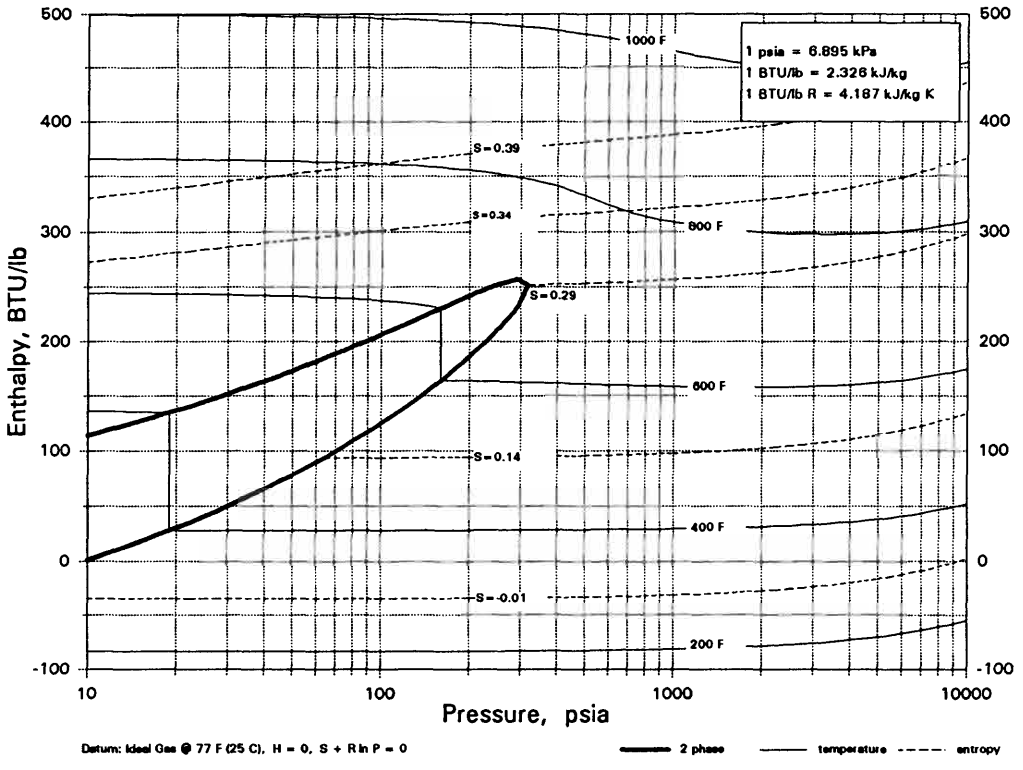
C10H20O2 2-ETHYLHEXYL ACETATE



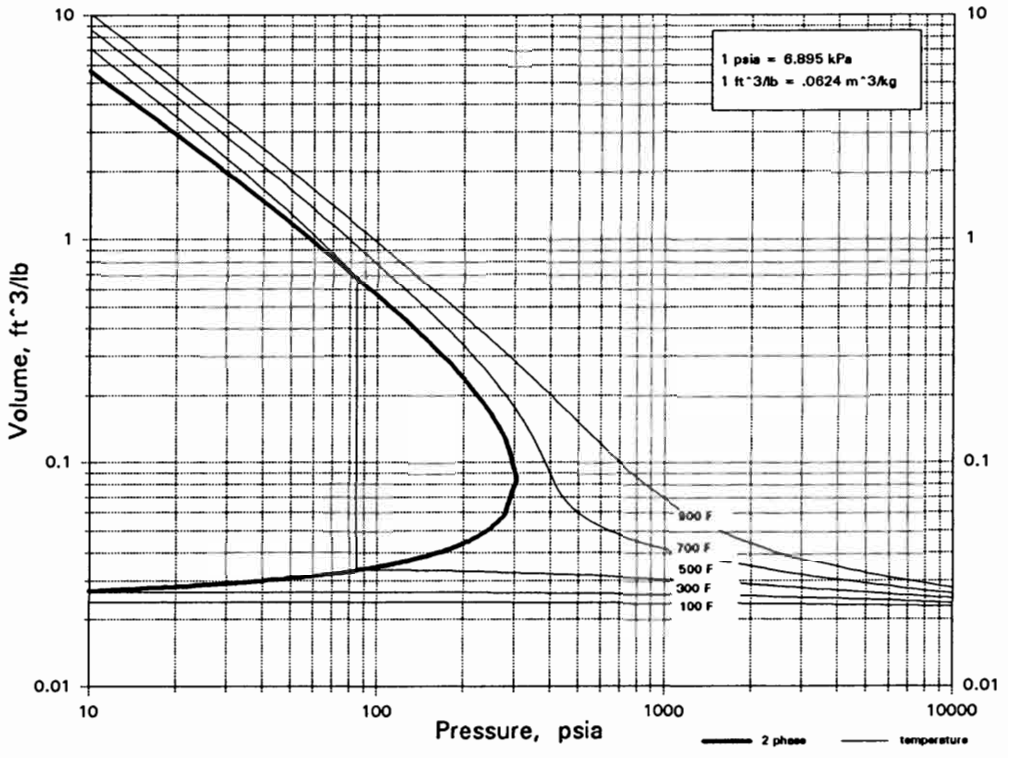


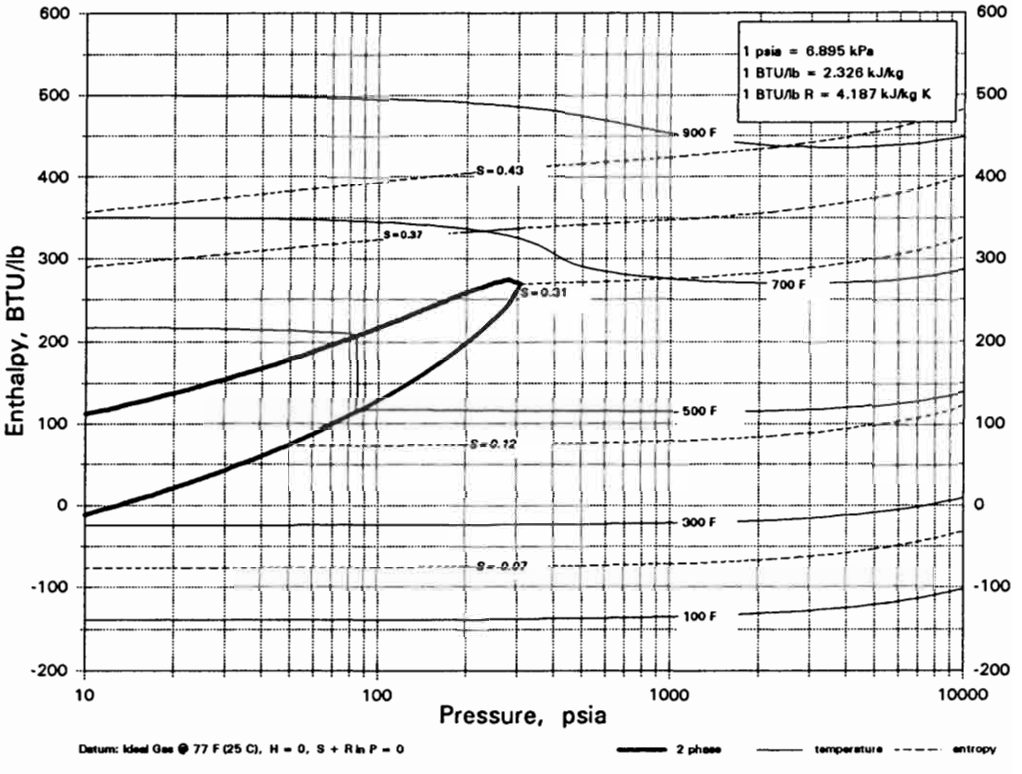
C10H20O2 ISOPENTYL ISOVALERATE



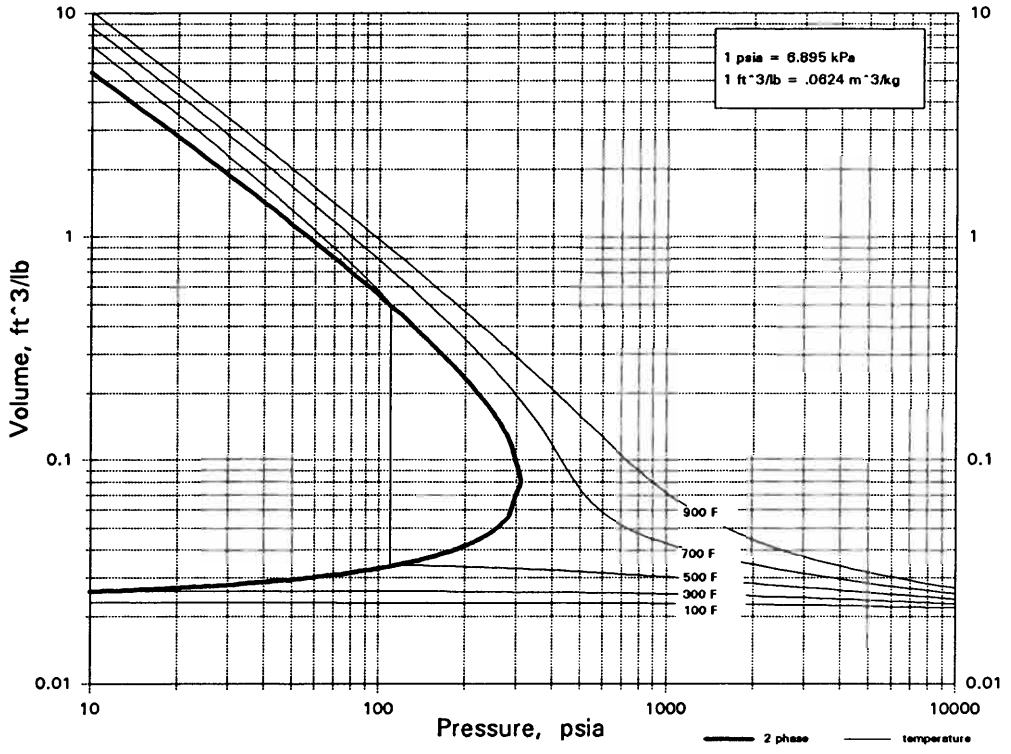


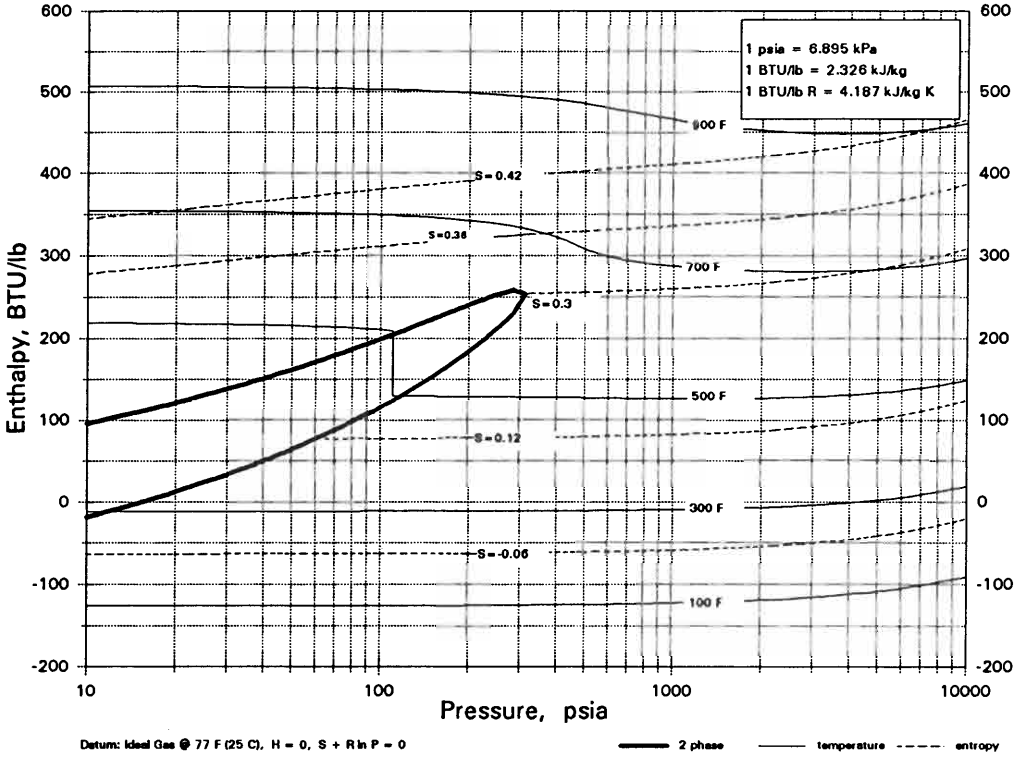
C10H22 n-DECANE



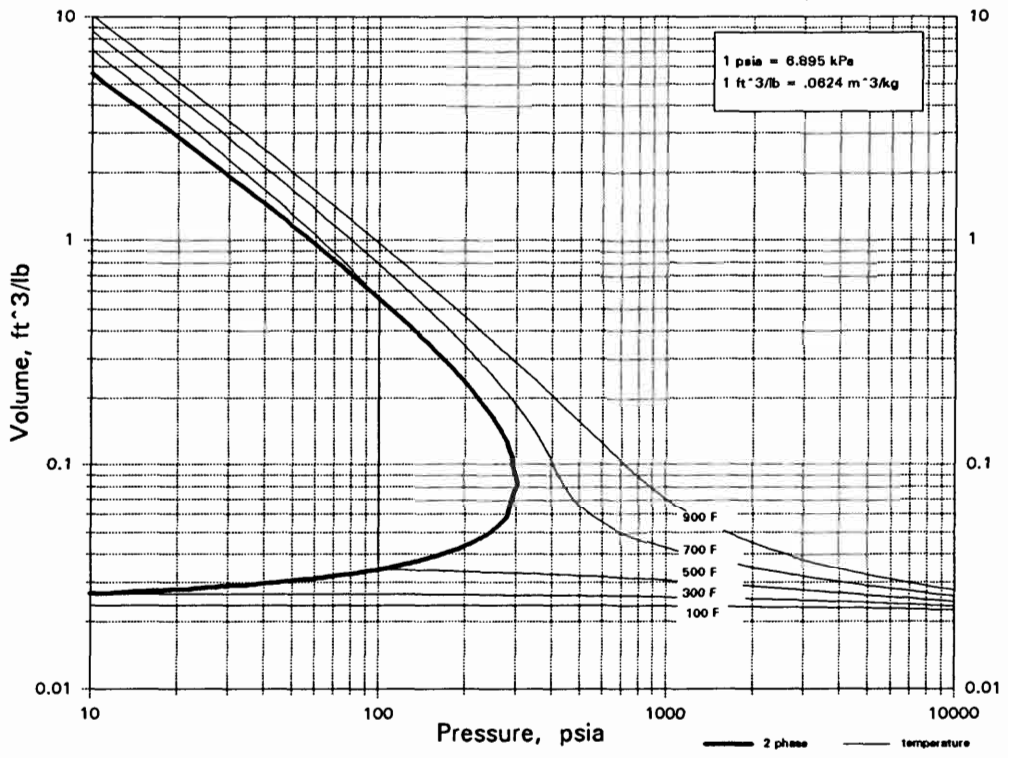


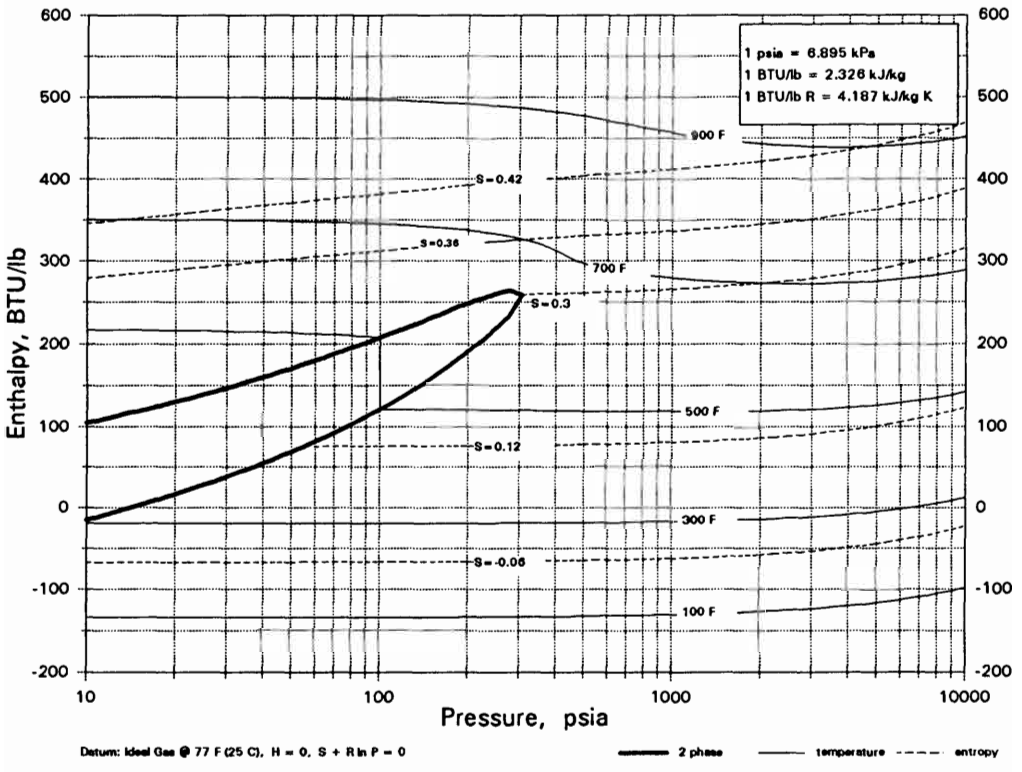
C10H22	2-2-DIMETHYLOCTANE



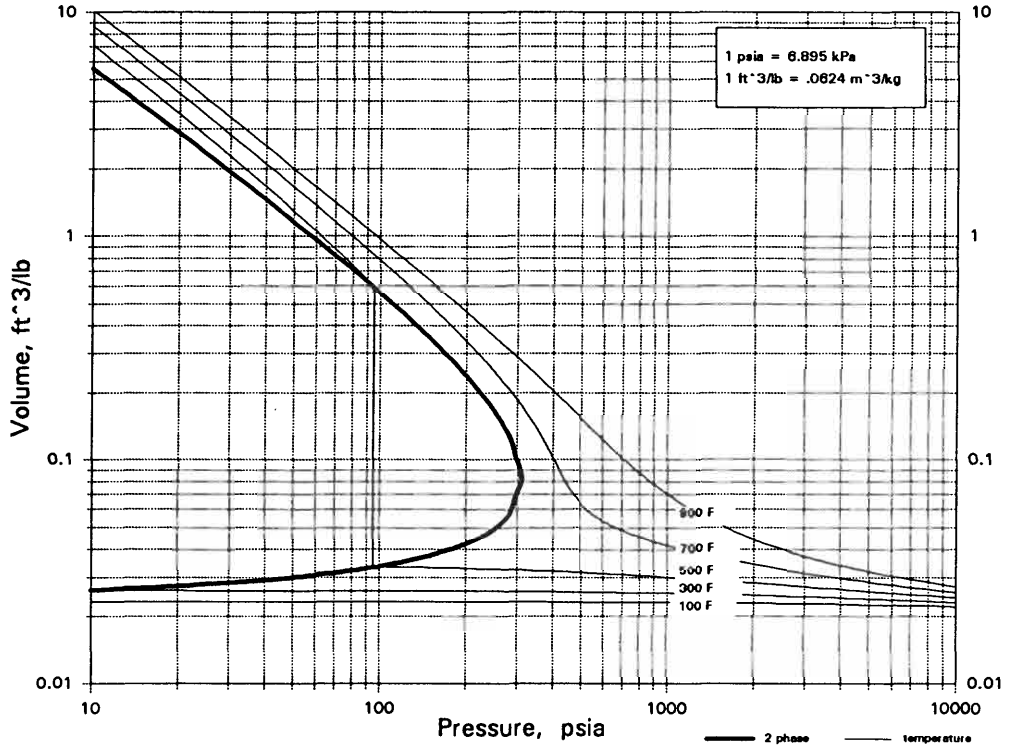


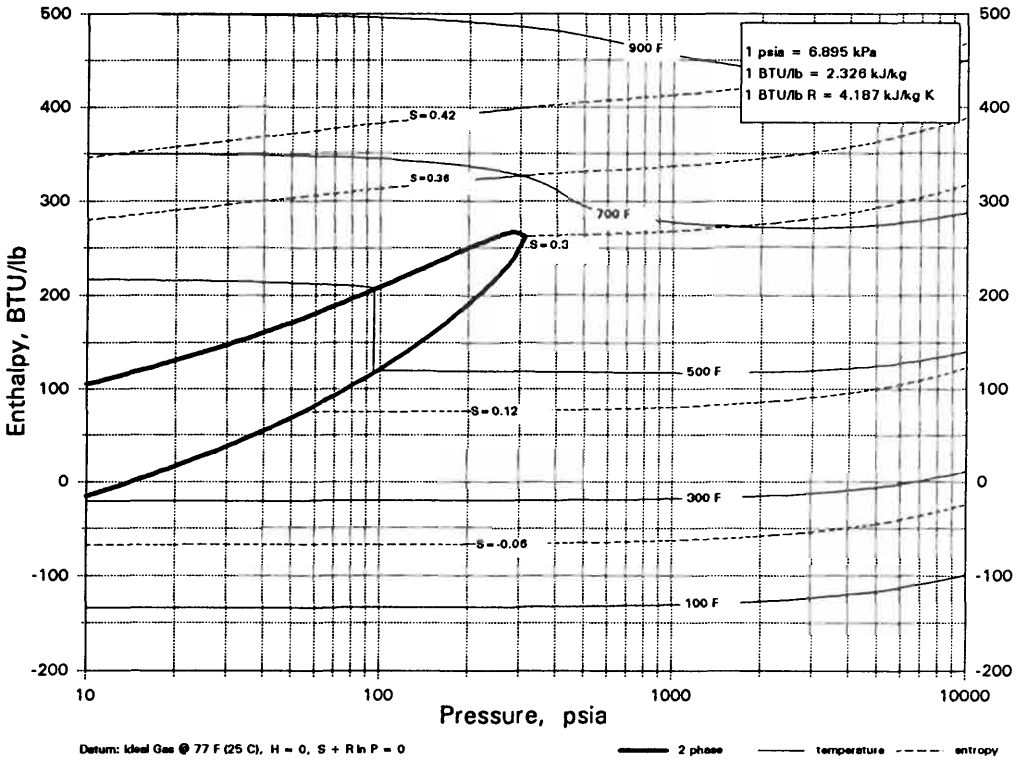
C10H22 2-METHYLNONANE



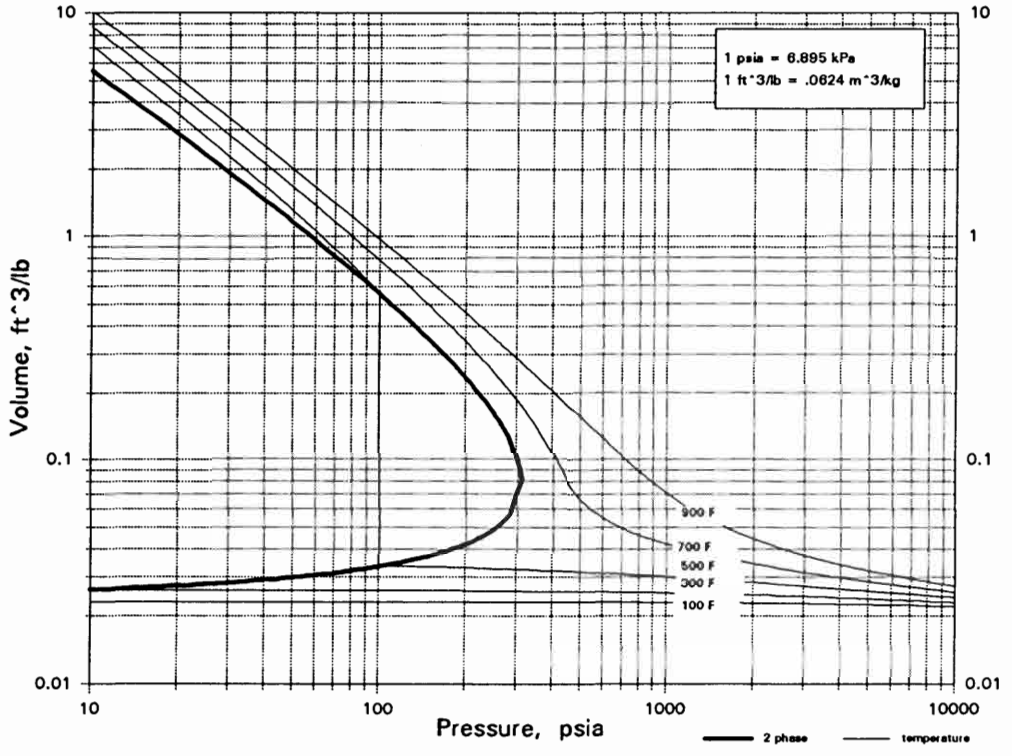


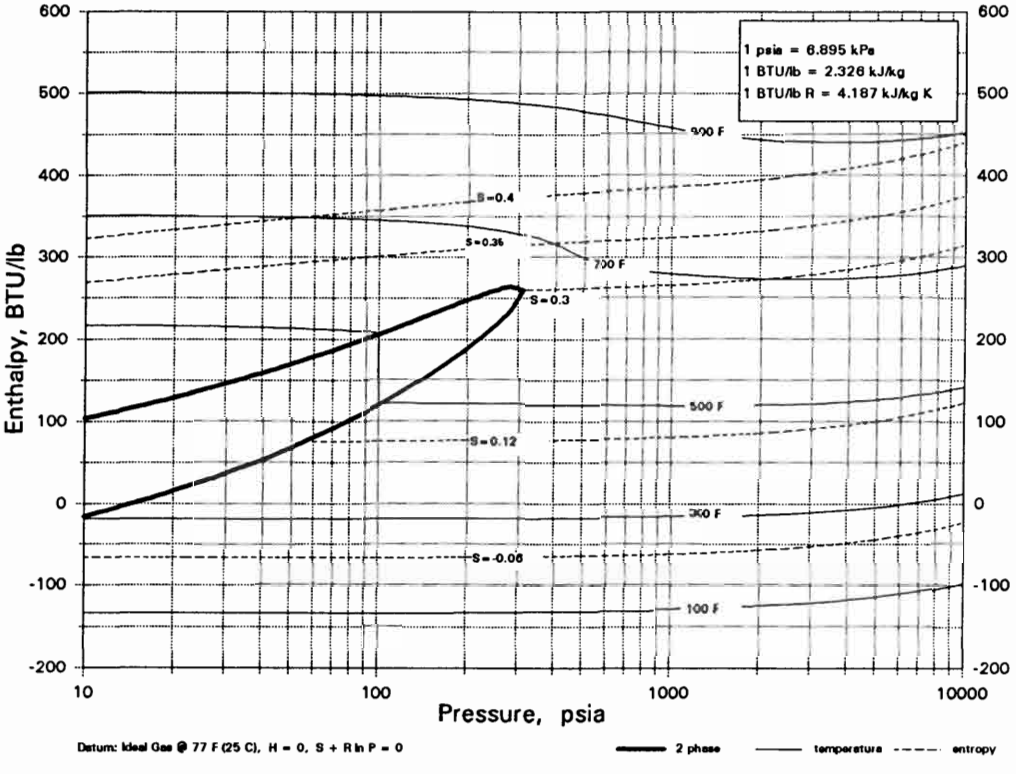
C10H22 3-METHYLNONANE



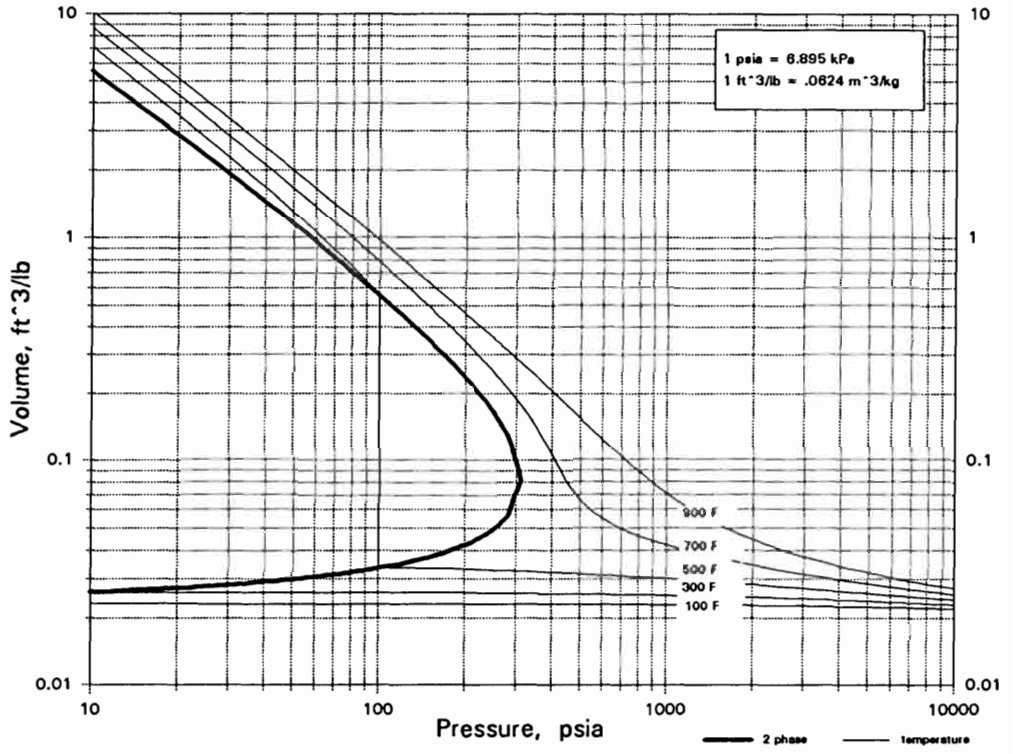


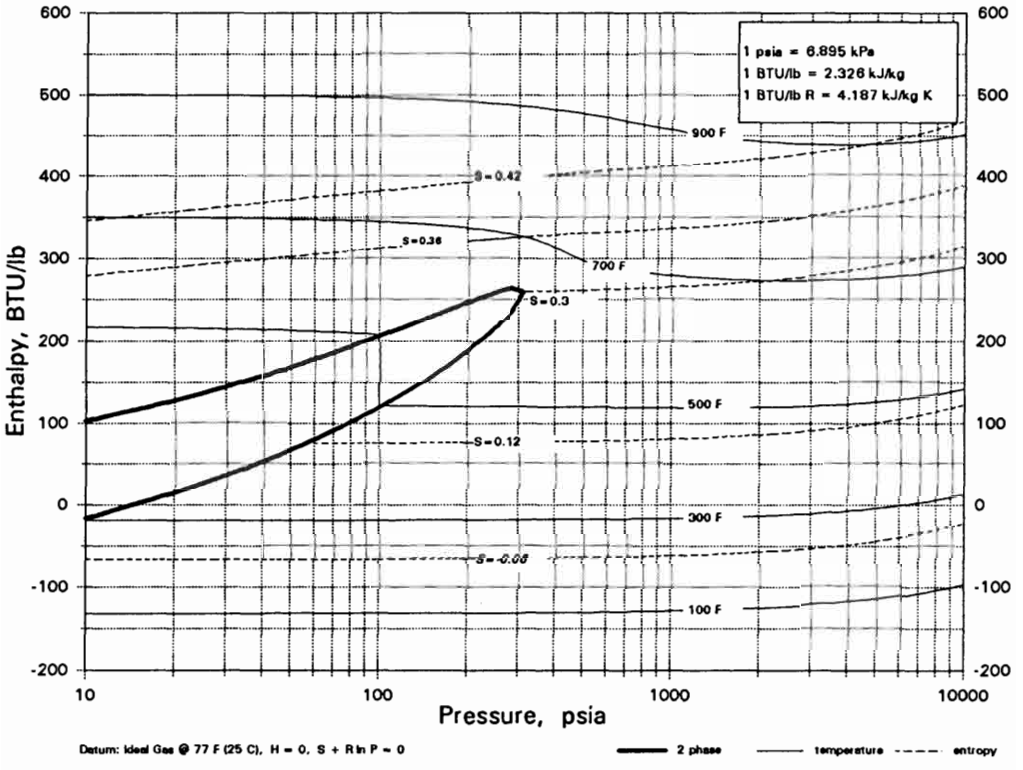
C10H22 4-METHYLNONANE



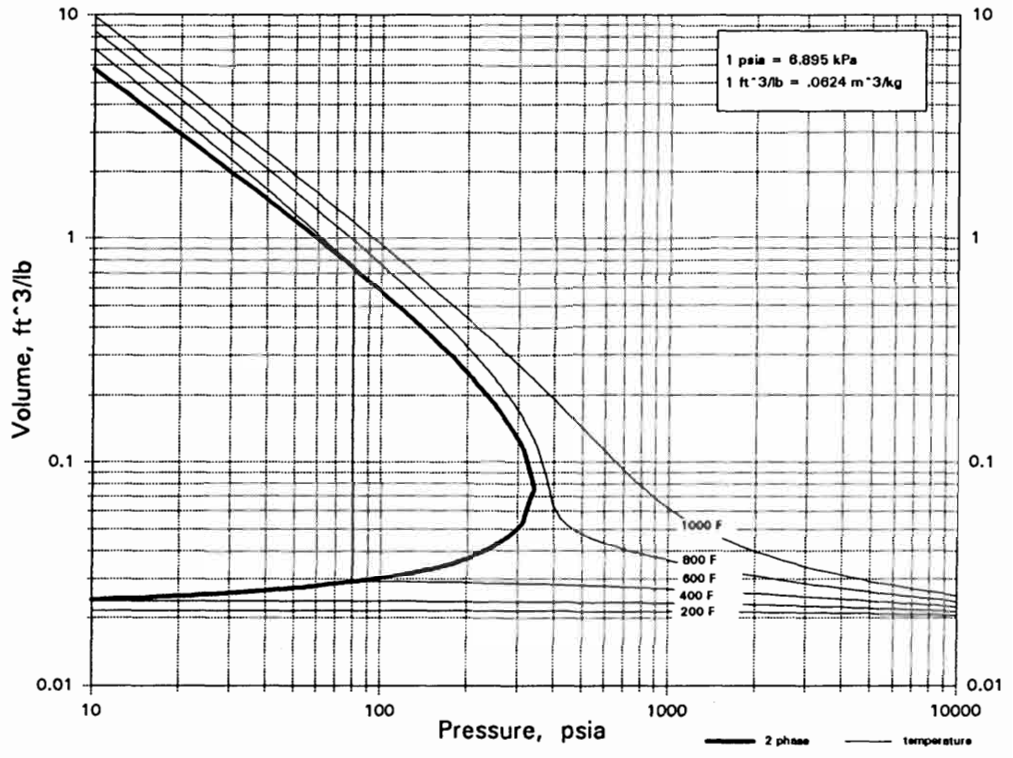


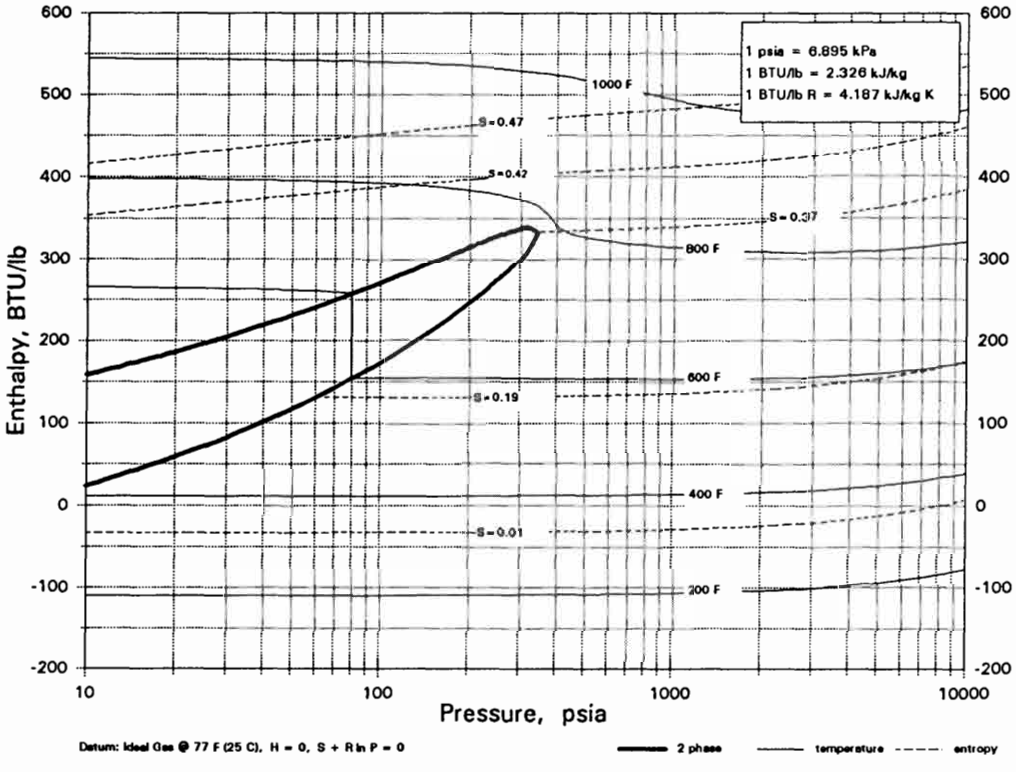
C10H22 5-METHYLNONANE



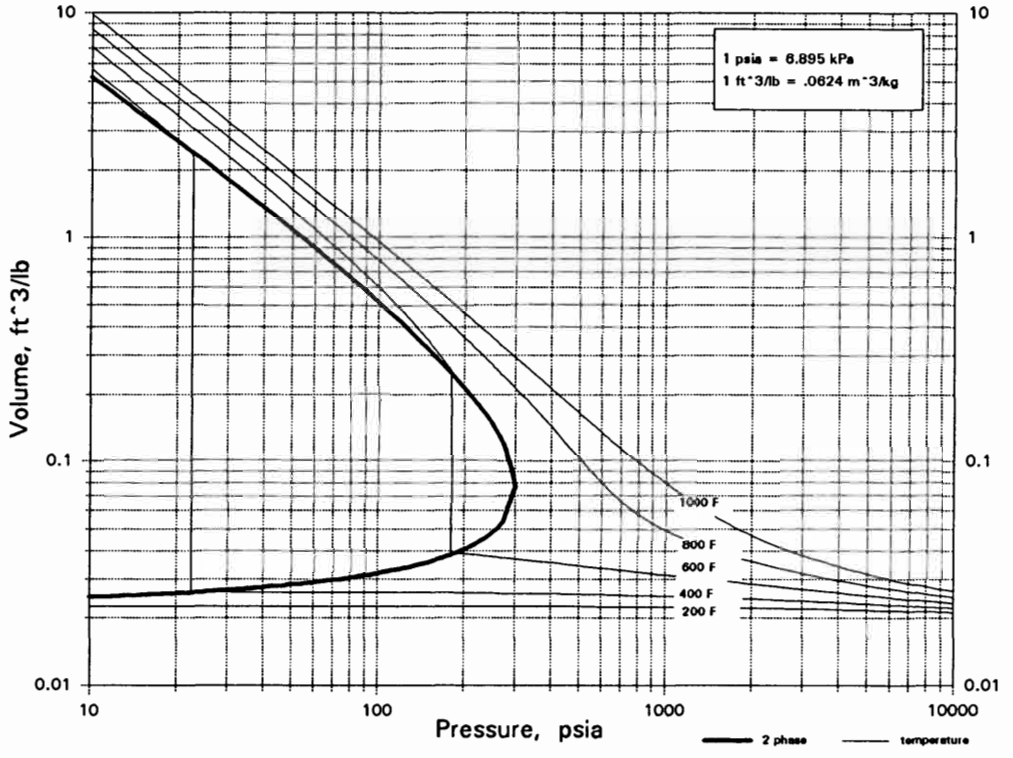


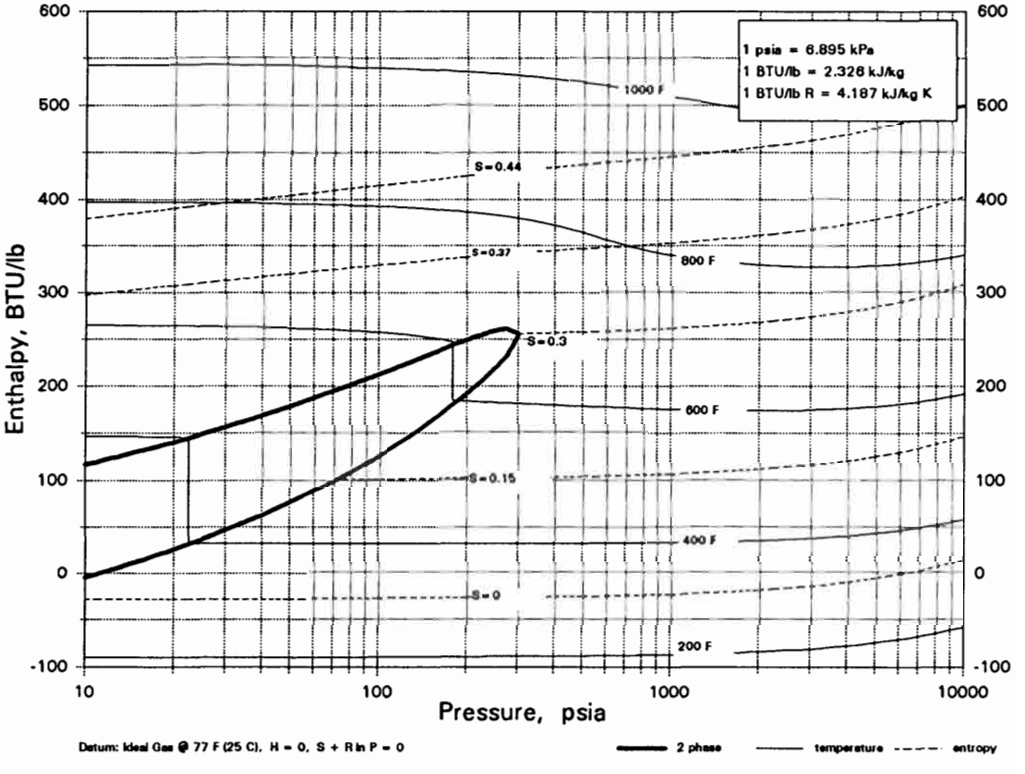
C10H22O 1-DECANOL



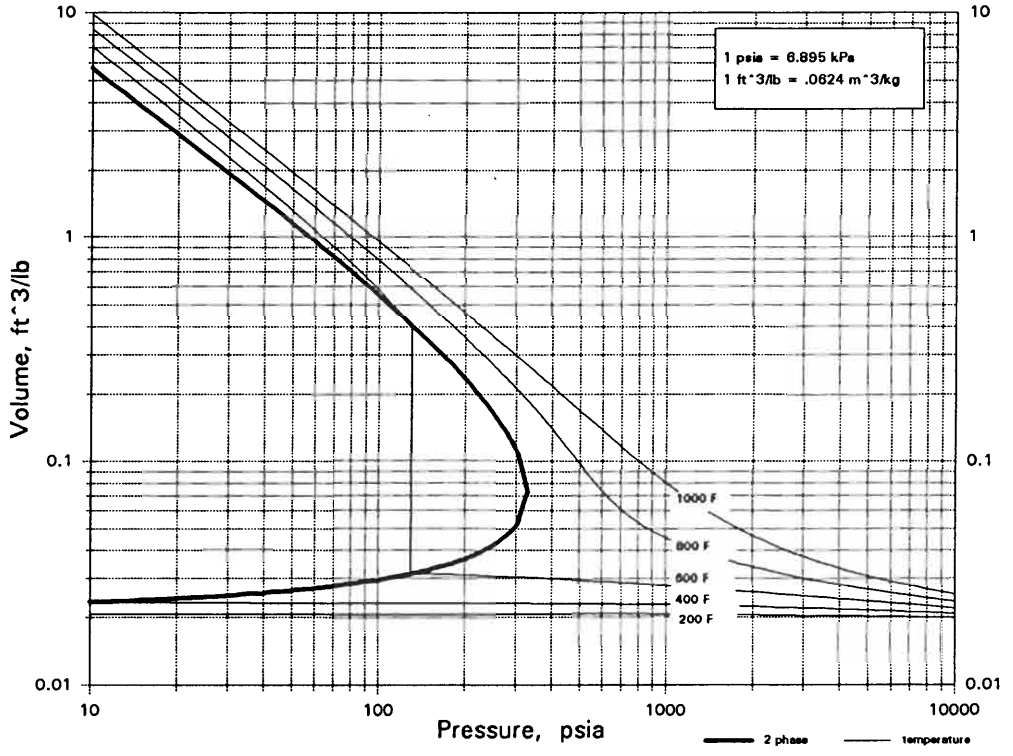


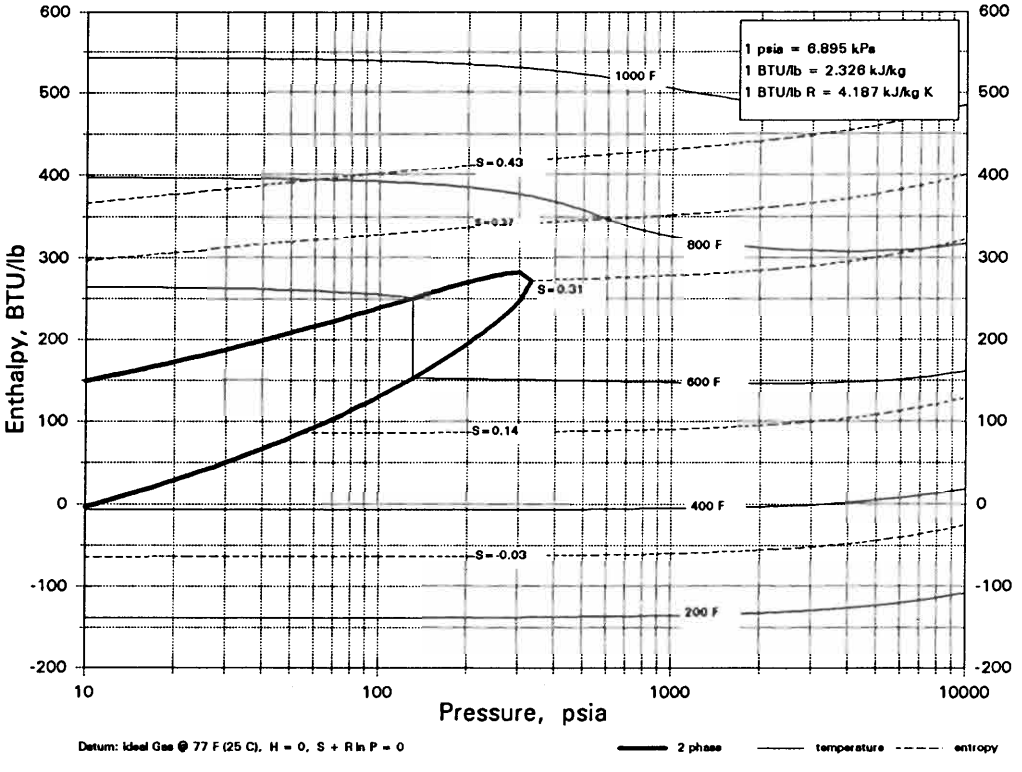
C10H22O DI-n-PENTYL ETHER



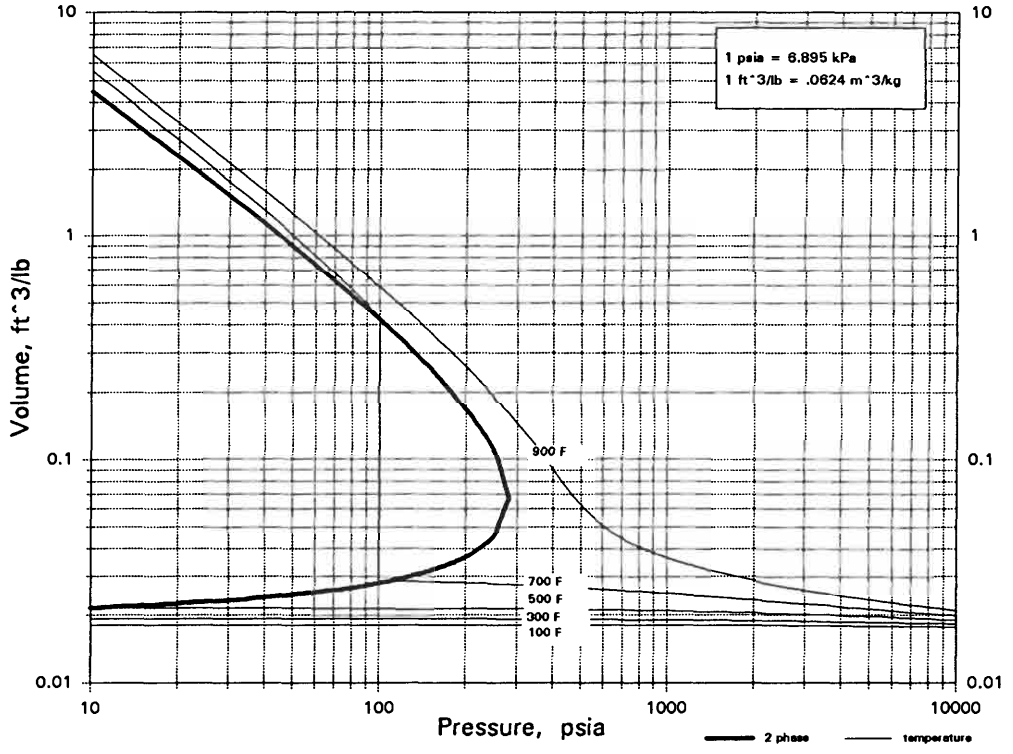


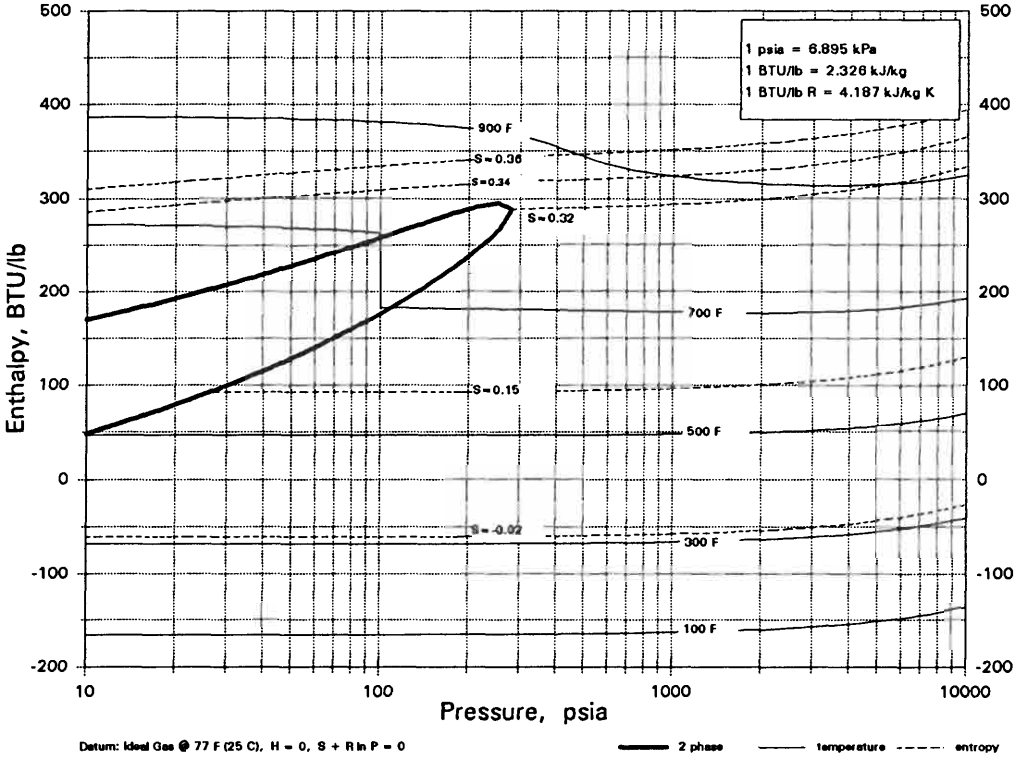
C10H22O ISODECANOL



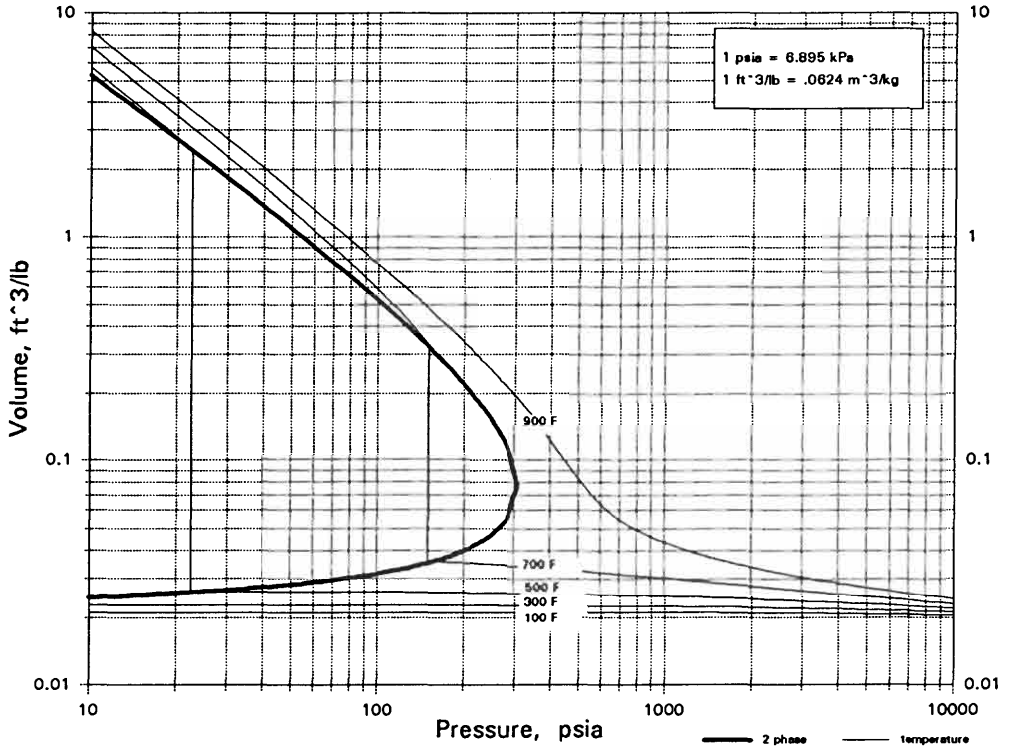


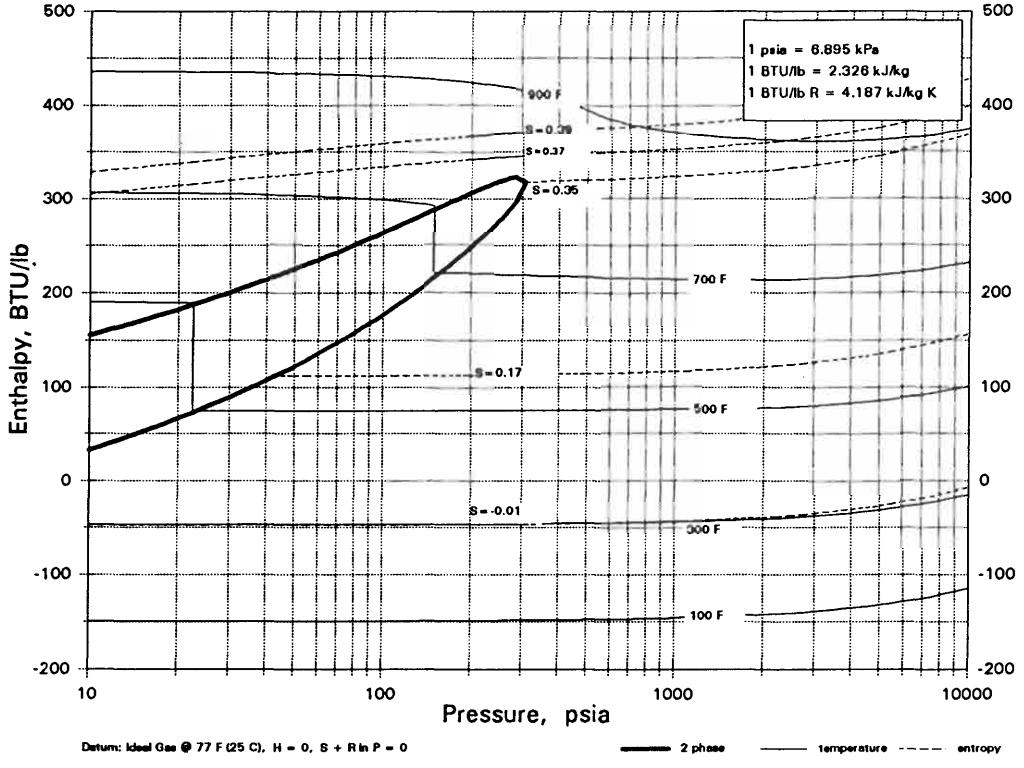
C10H22O5 TETRAETHYLENE GLYCOL DIMETHYL ETHER



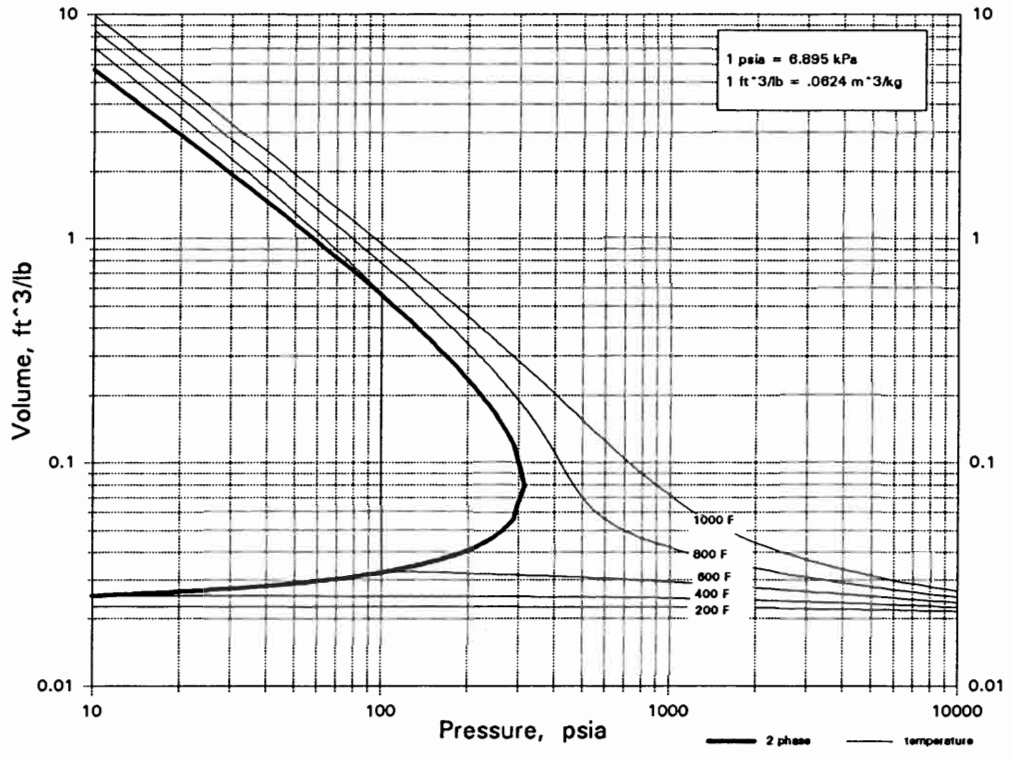


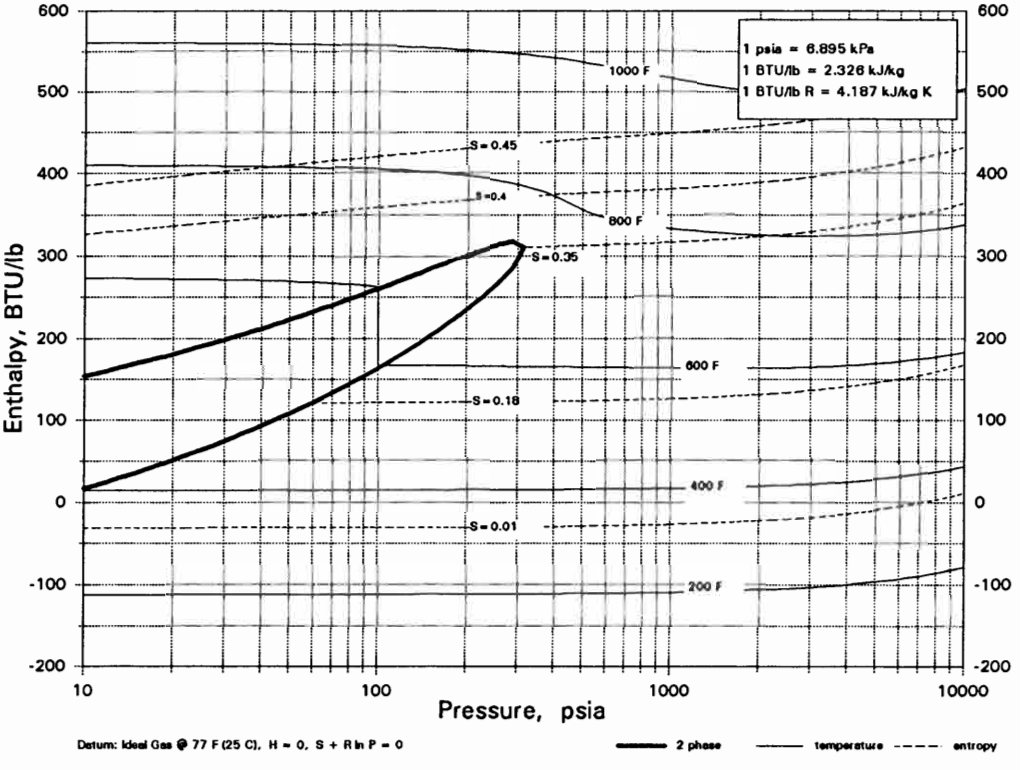
C10H22S n-DECYL MERCAPTAN



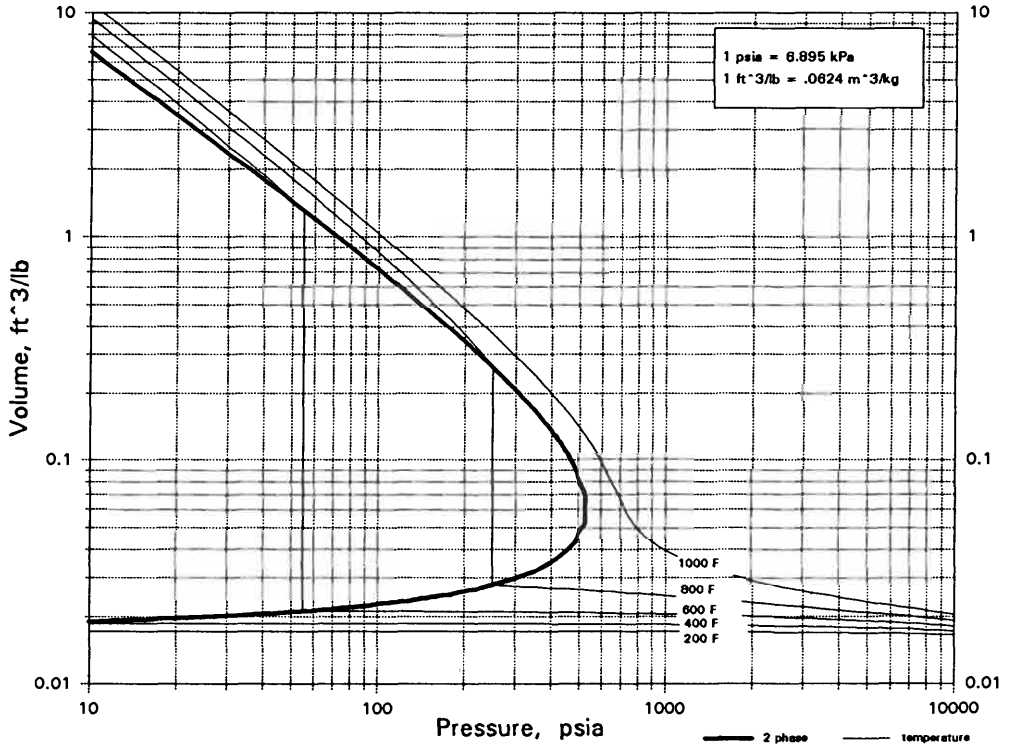


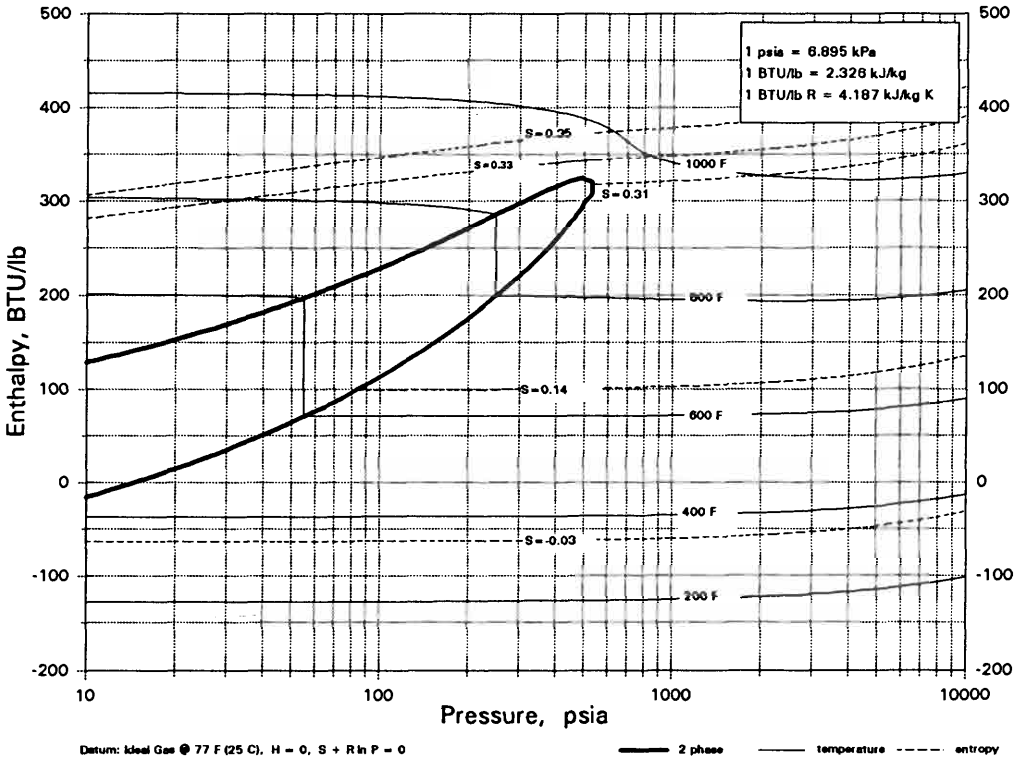
C10H23N n-DECYLAMINE



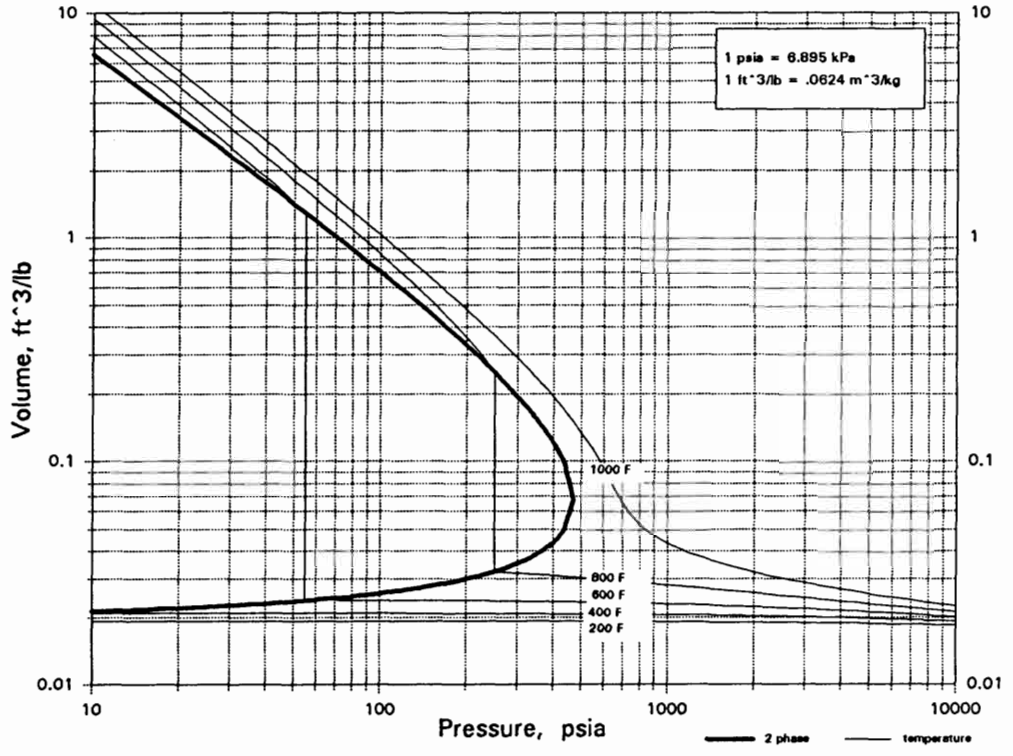


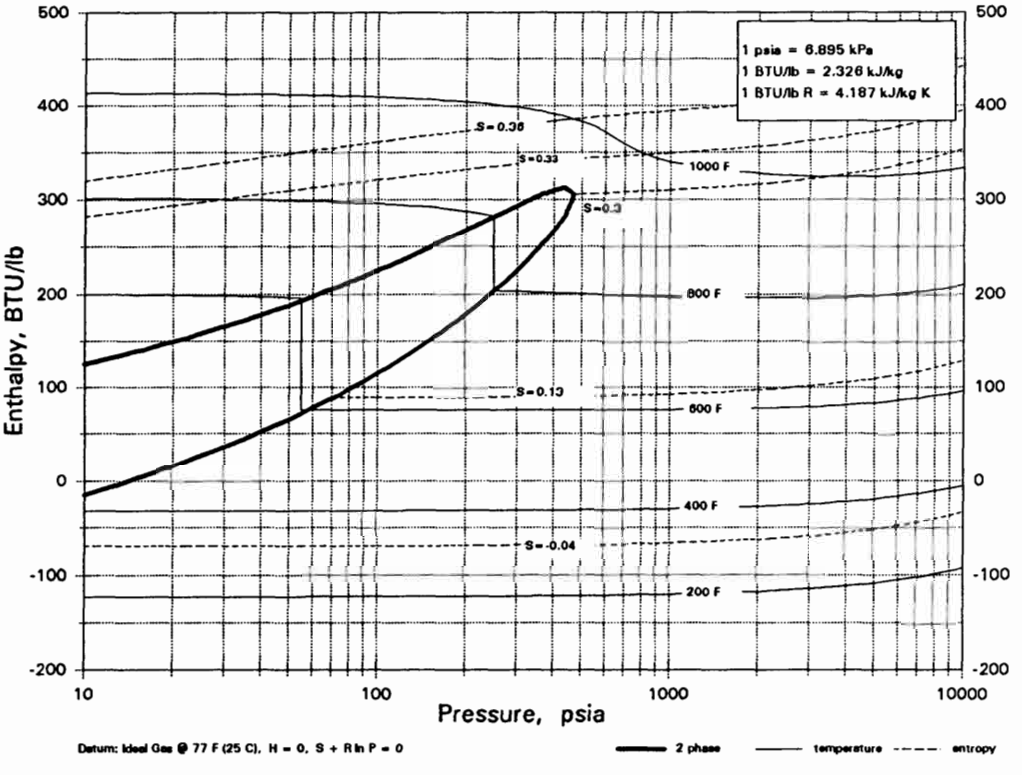
C11H10 1-METHYLNAPHTHALENE



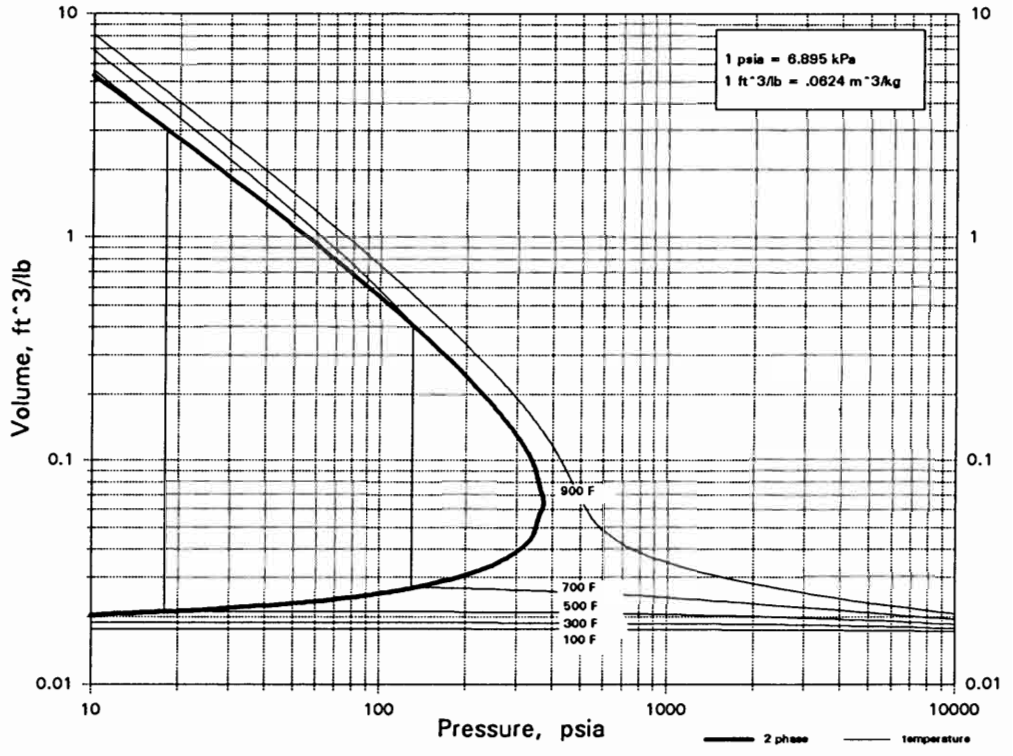


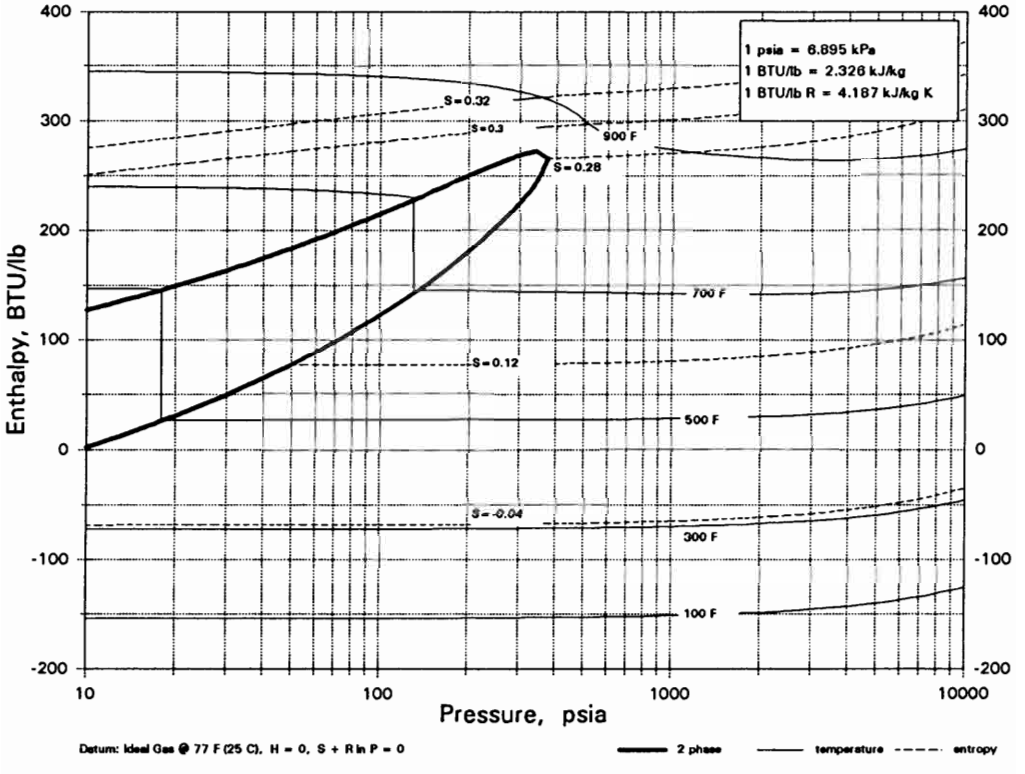
C11H10 2-METHYLNAPHTHALENE



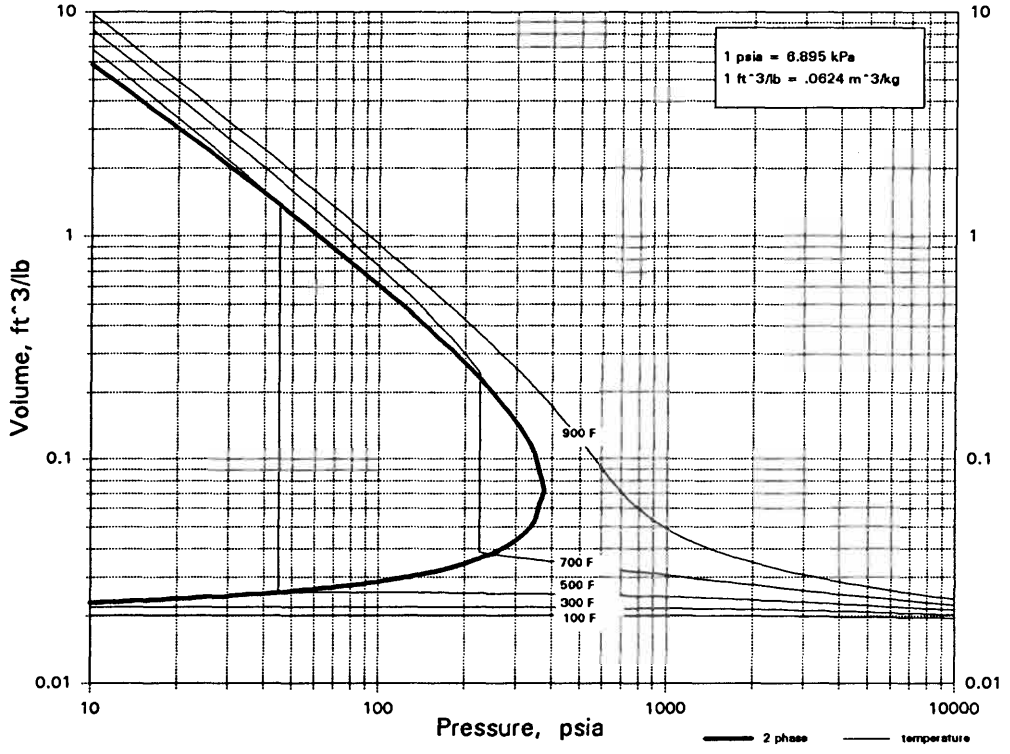


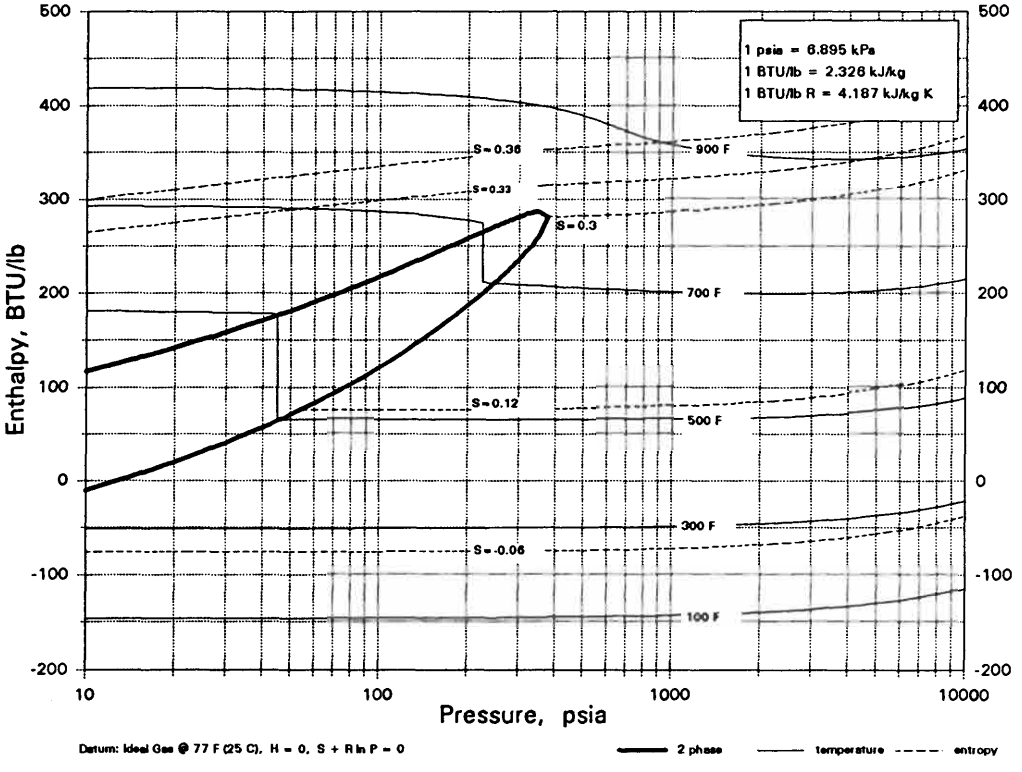
C11H14O2 n-BUTYL BENZOATE



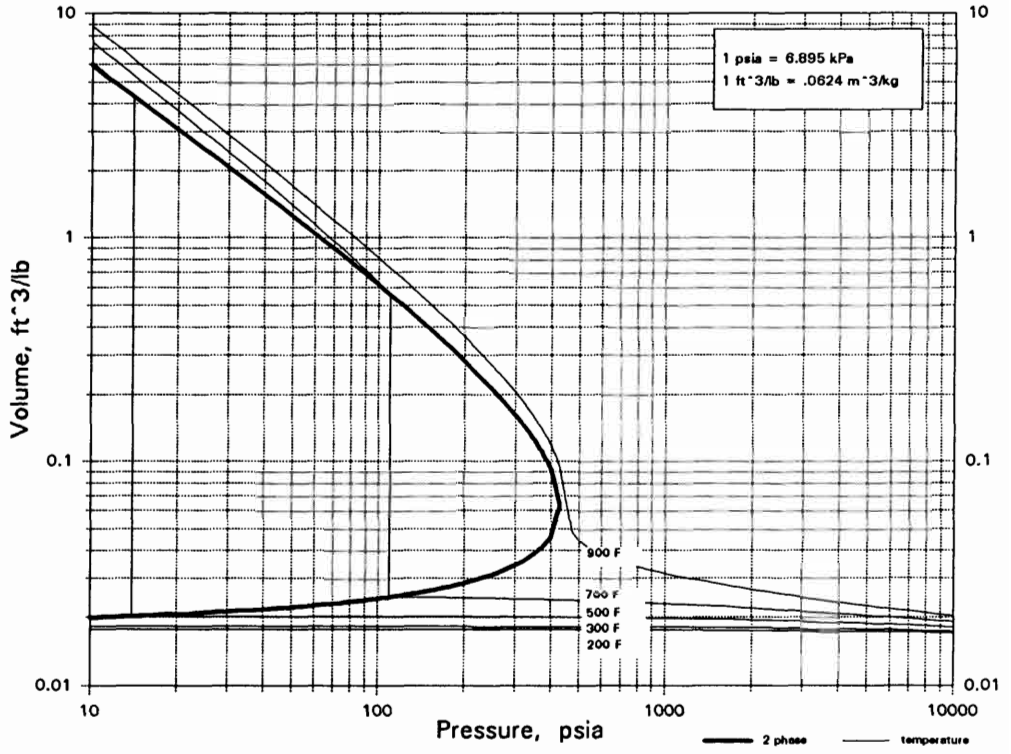


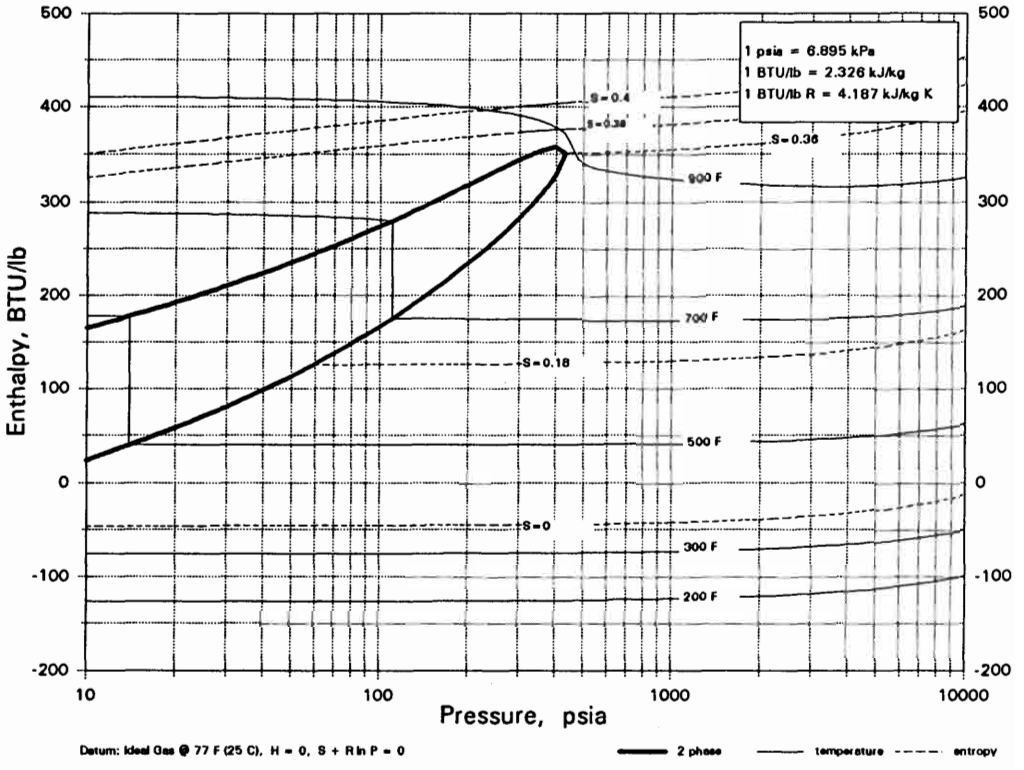
C11H16 n-PENTYLBENZENE



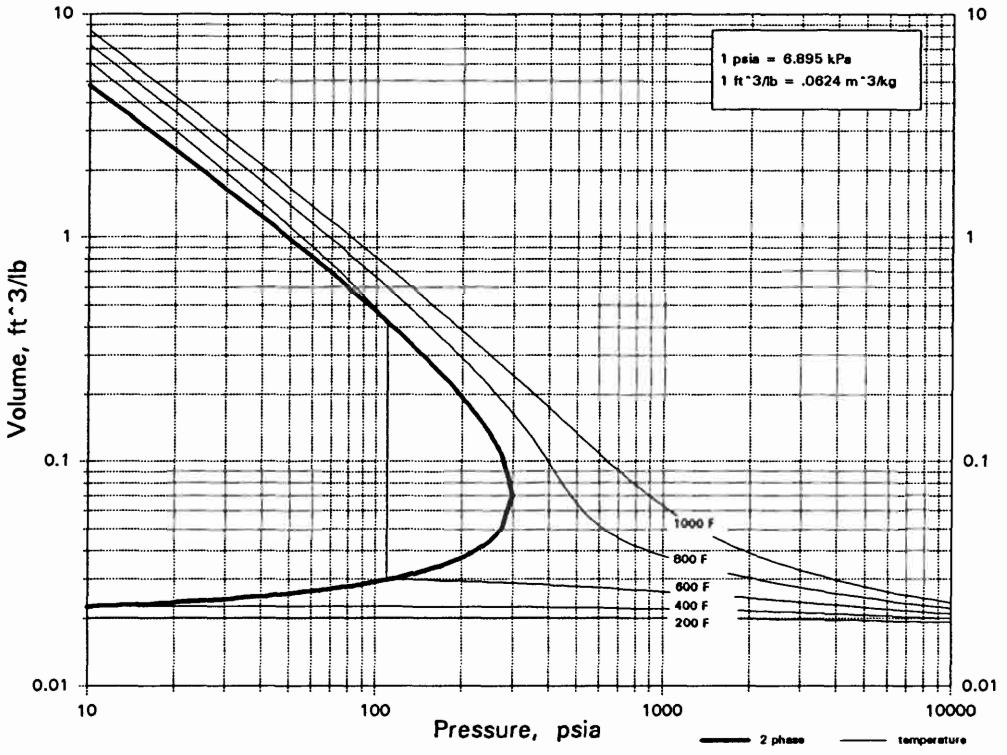


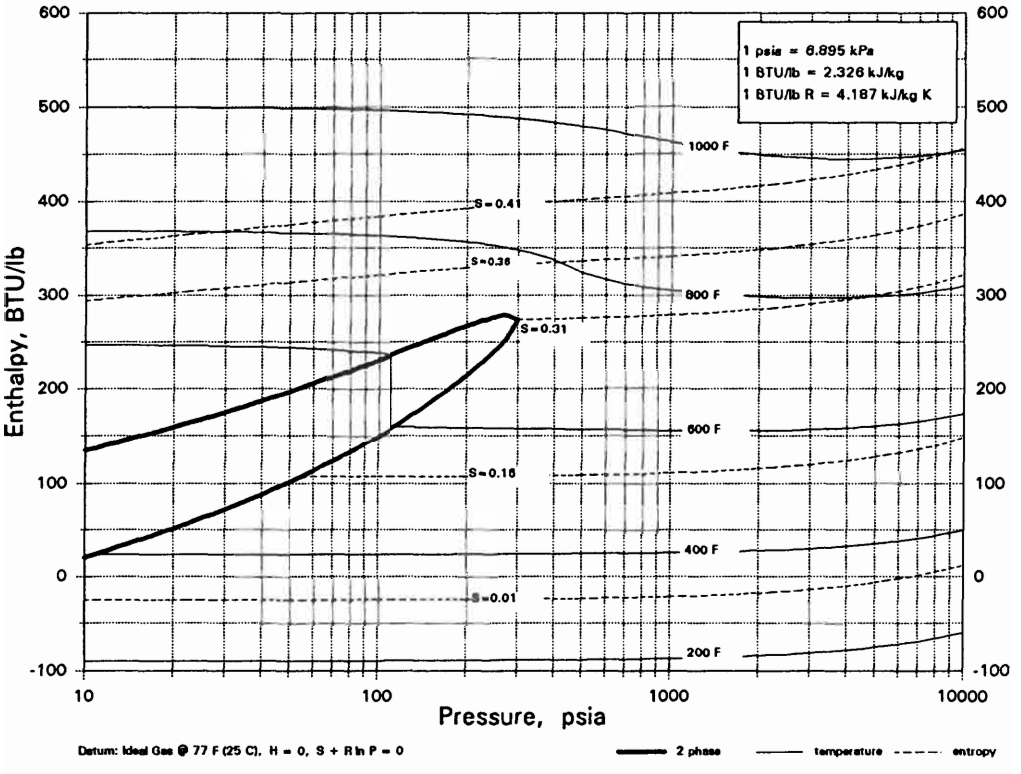
C11H16O p-tert-AMYLPHENOL



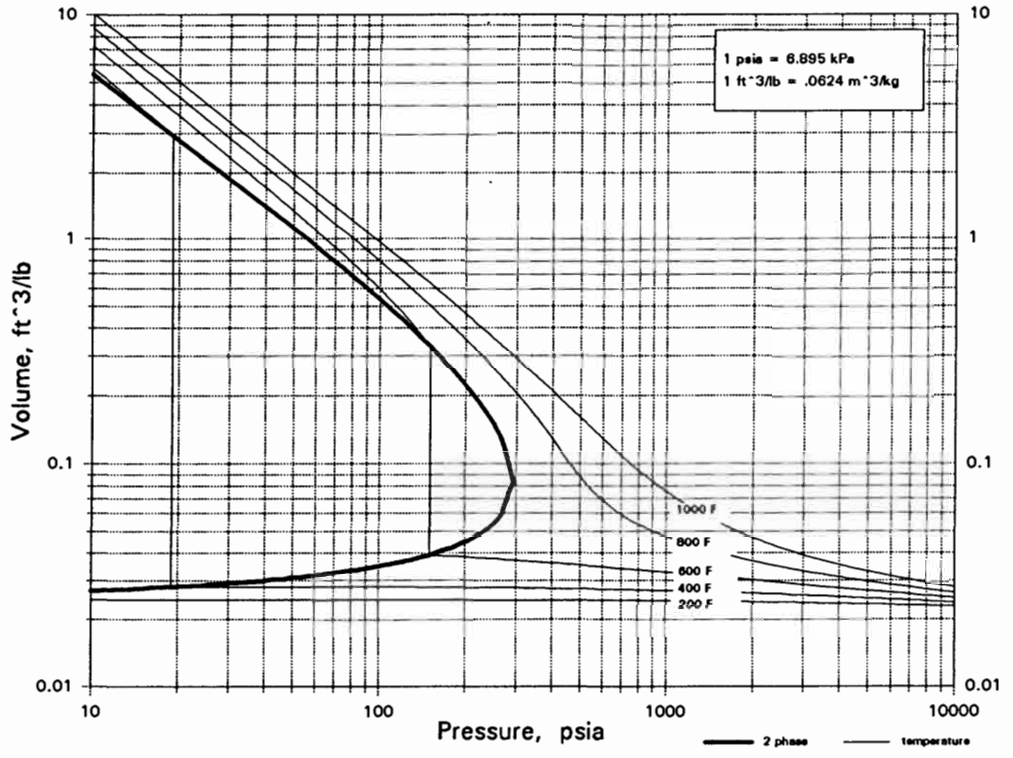


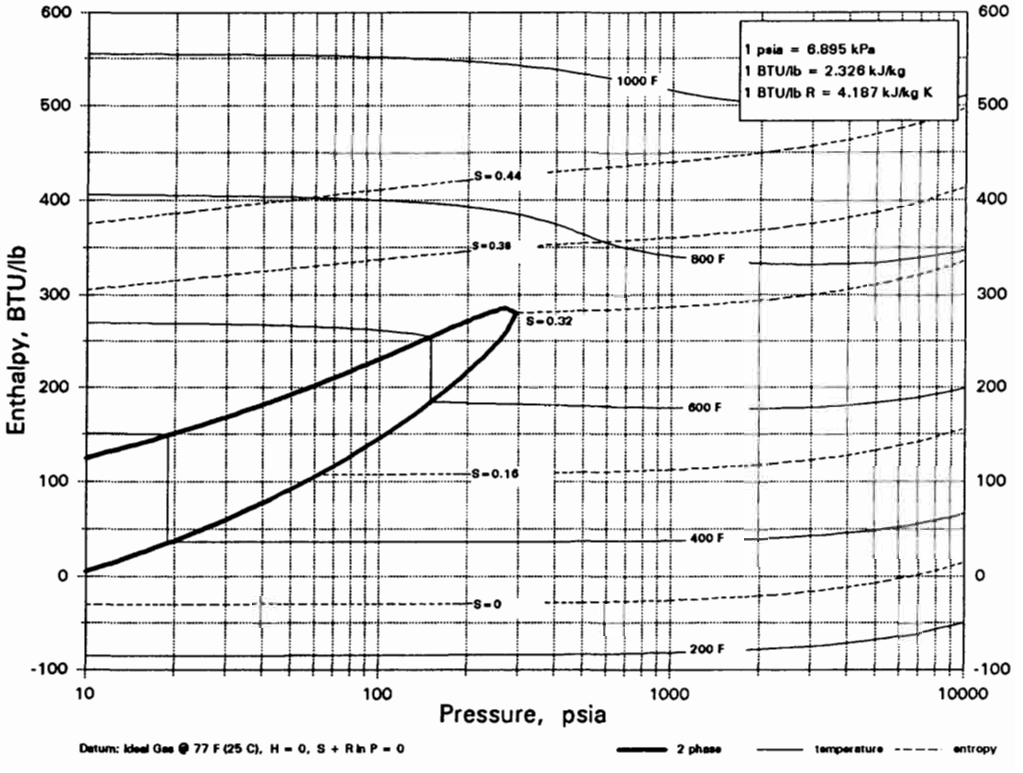
C11H20O2 2-ETHYLHEXYL ACRYLATE



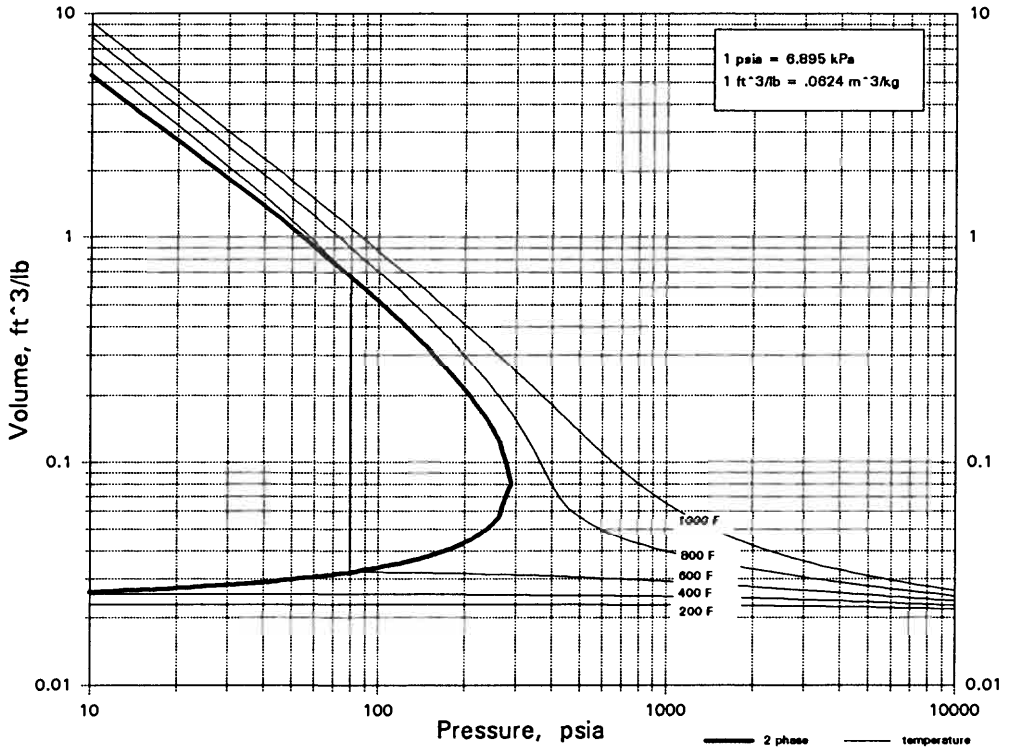


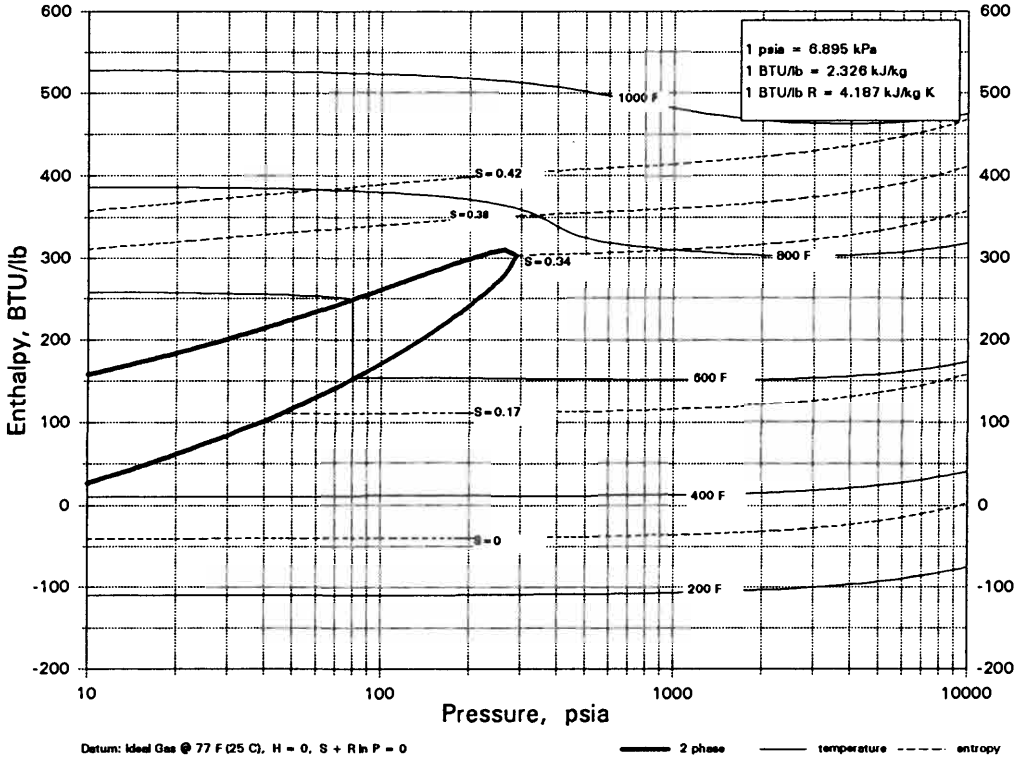
C11H22 1-UNDECENE



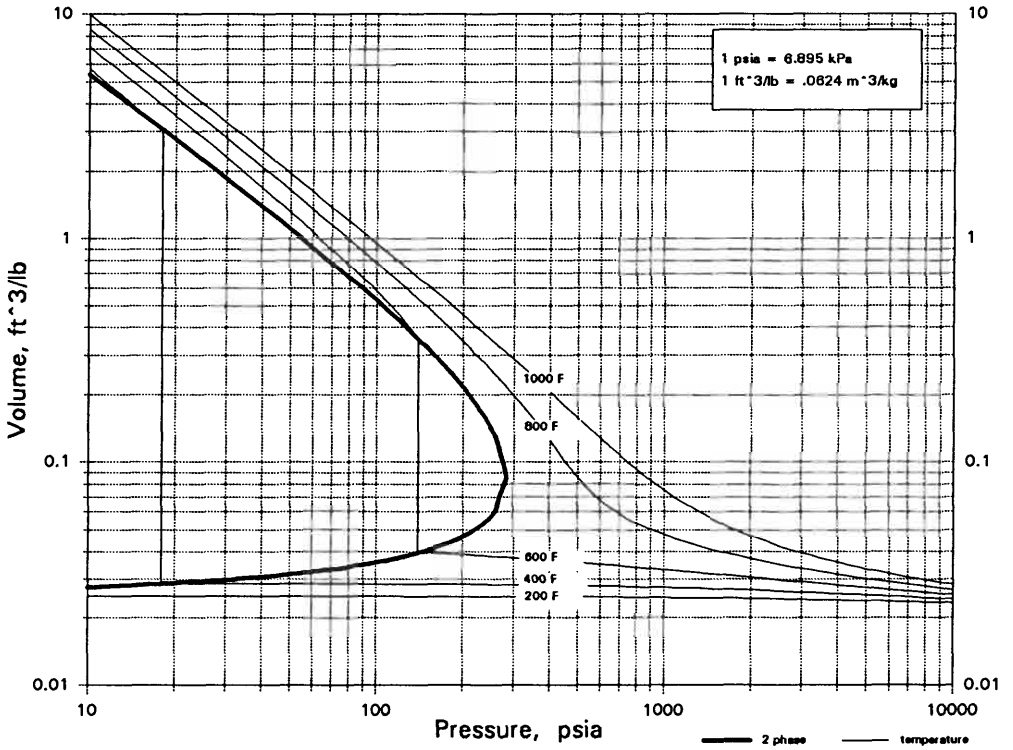


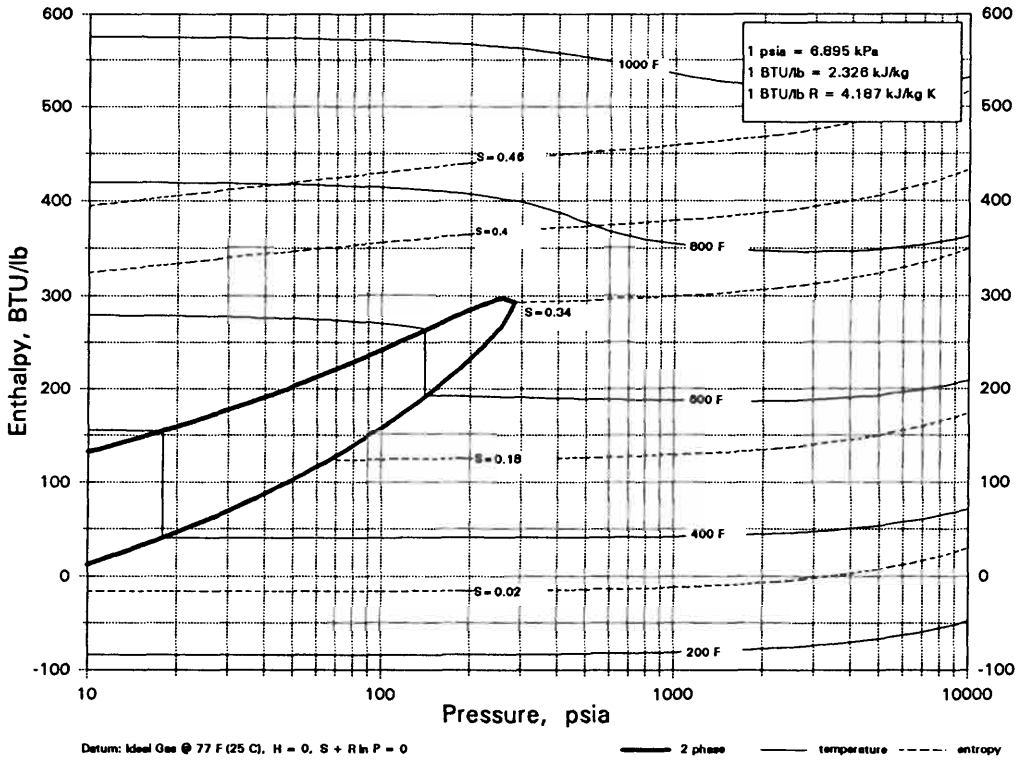
C11H22O 1-UNDECANAL



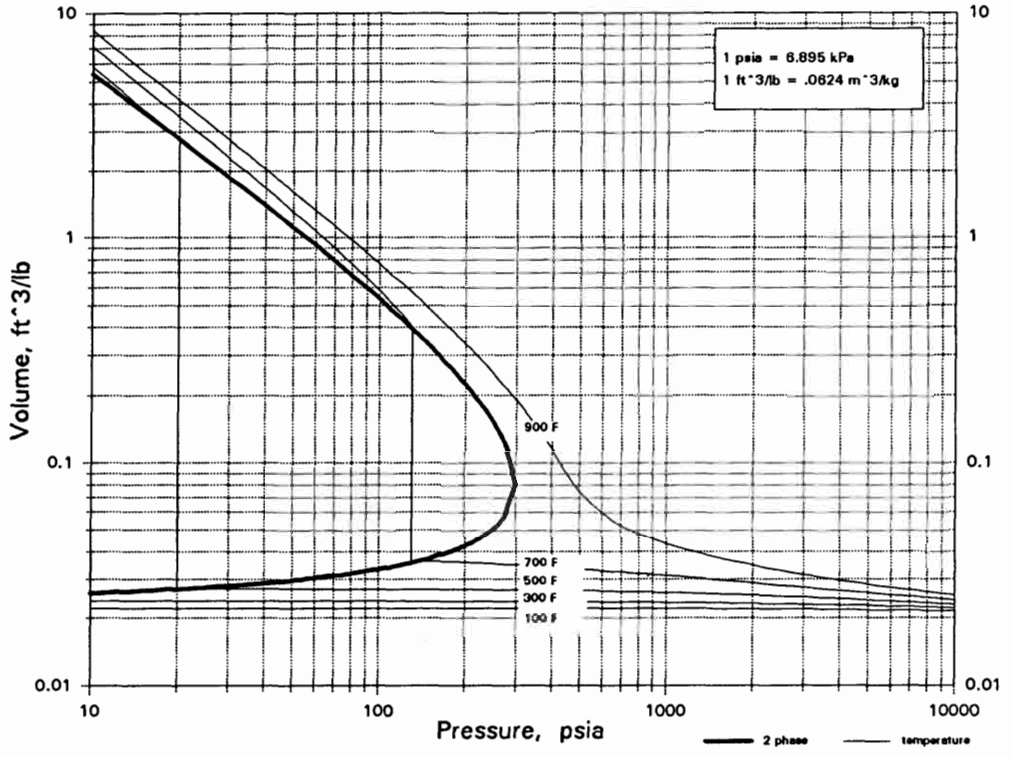


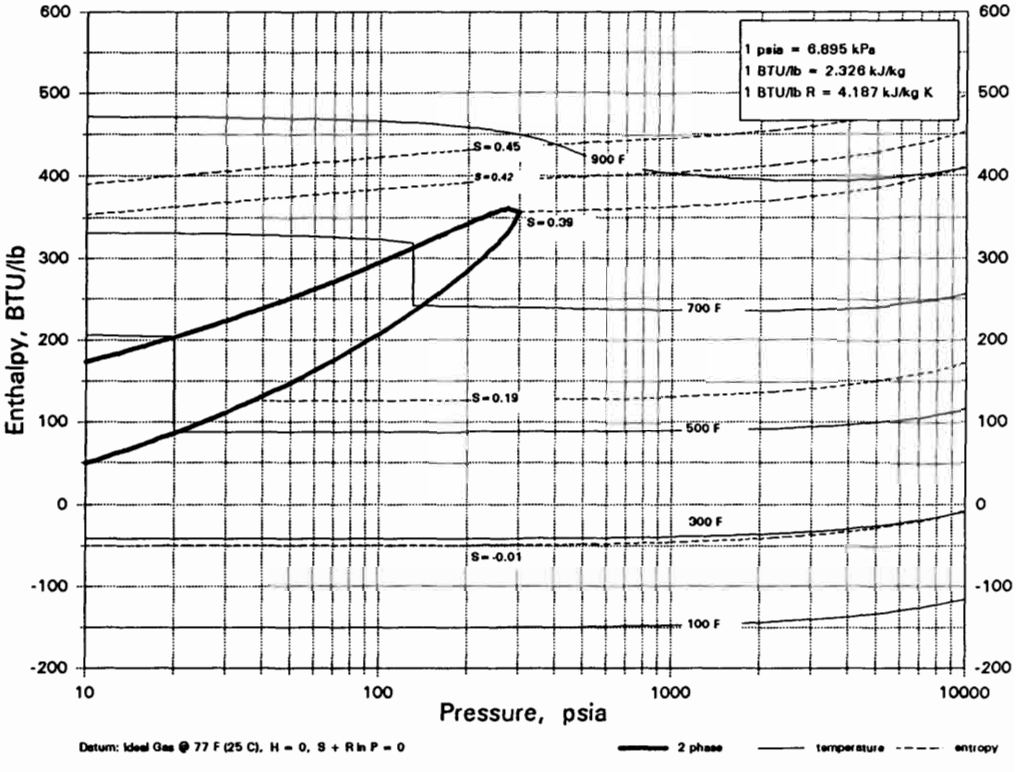
C11H24 n-UNDECANE



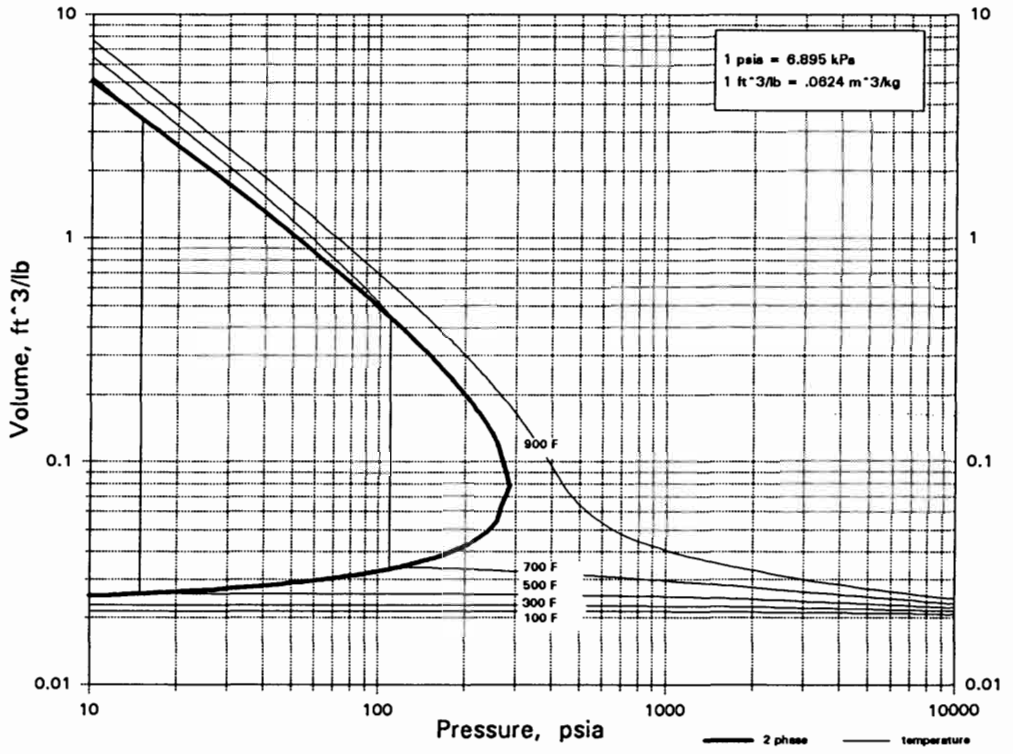


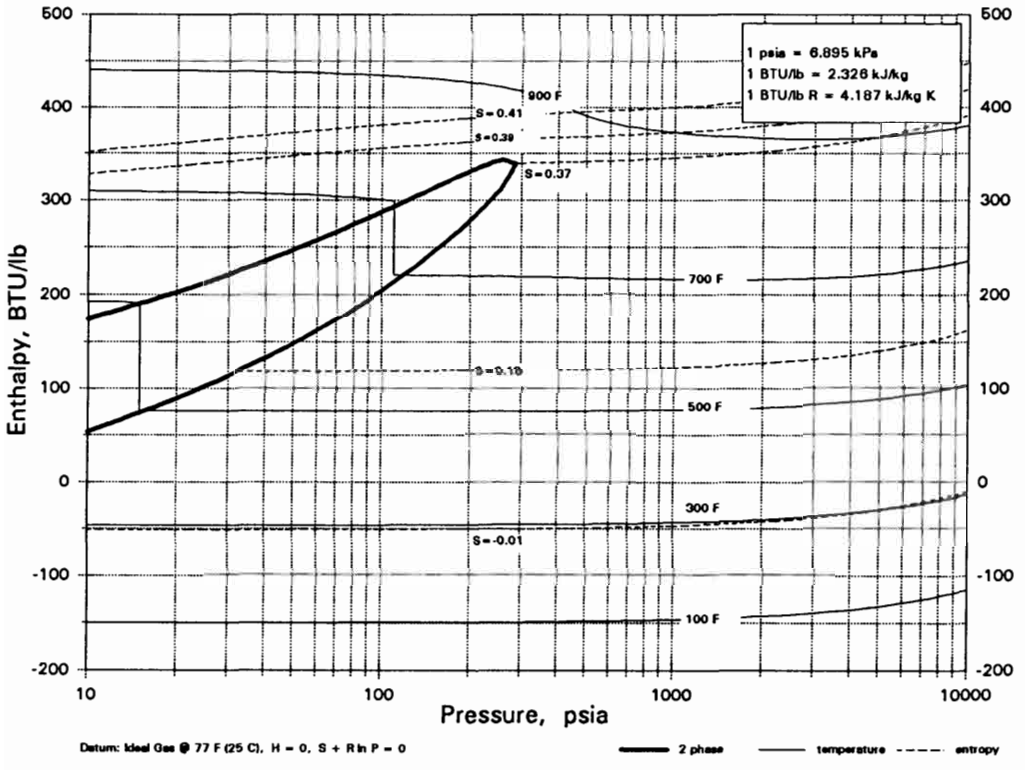
C11H24O 1-UNDECANOL



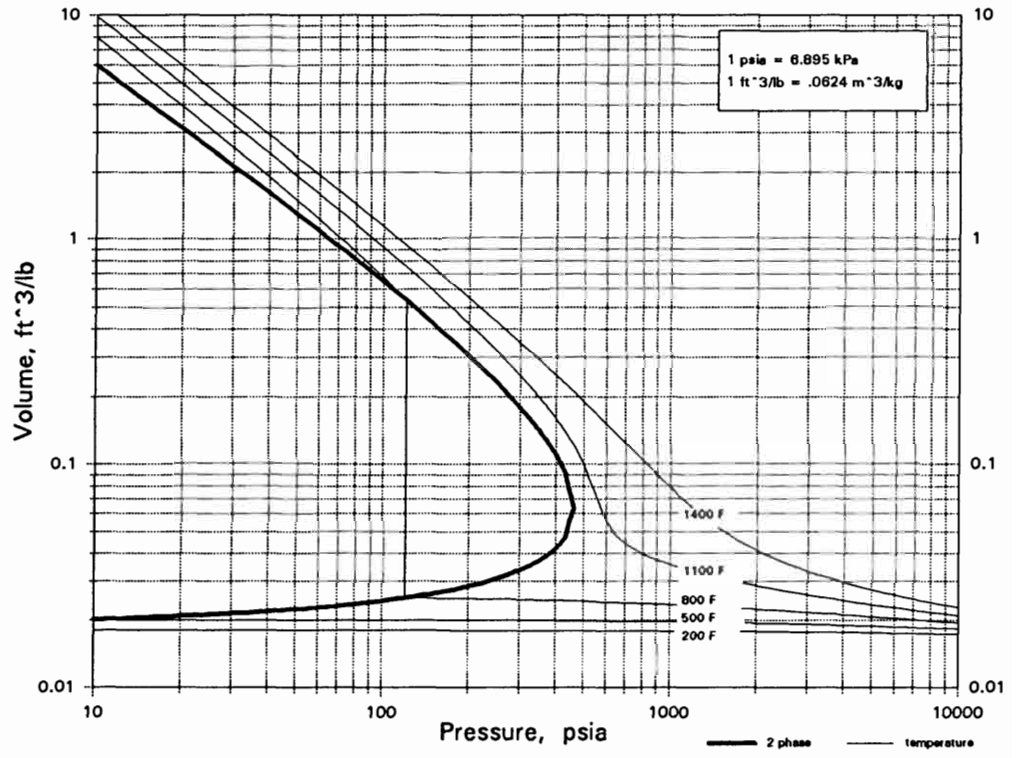


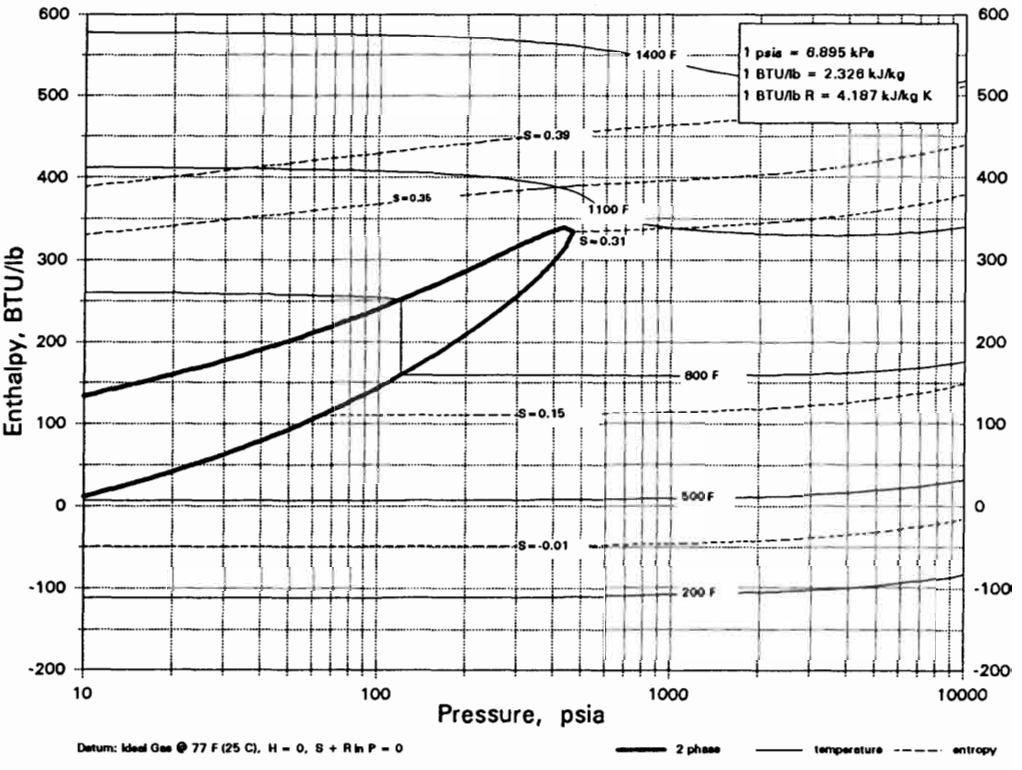
C11H24S UNDECYL MERCAPTAN



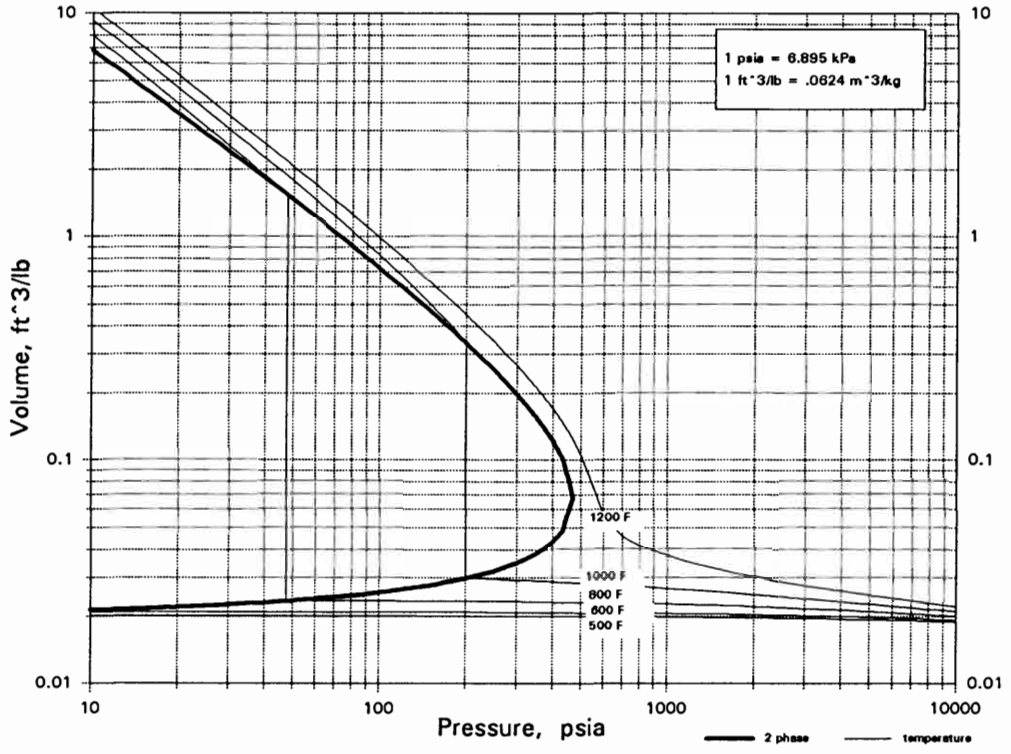


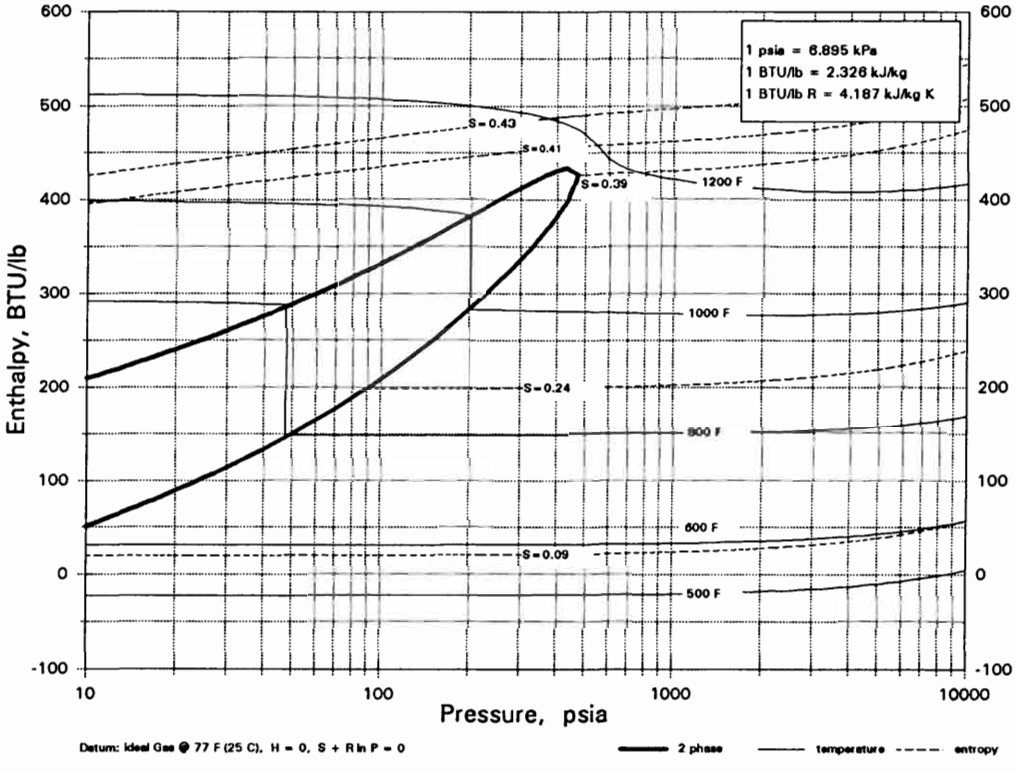
C12H8O DIBENZOFURAN



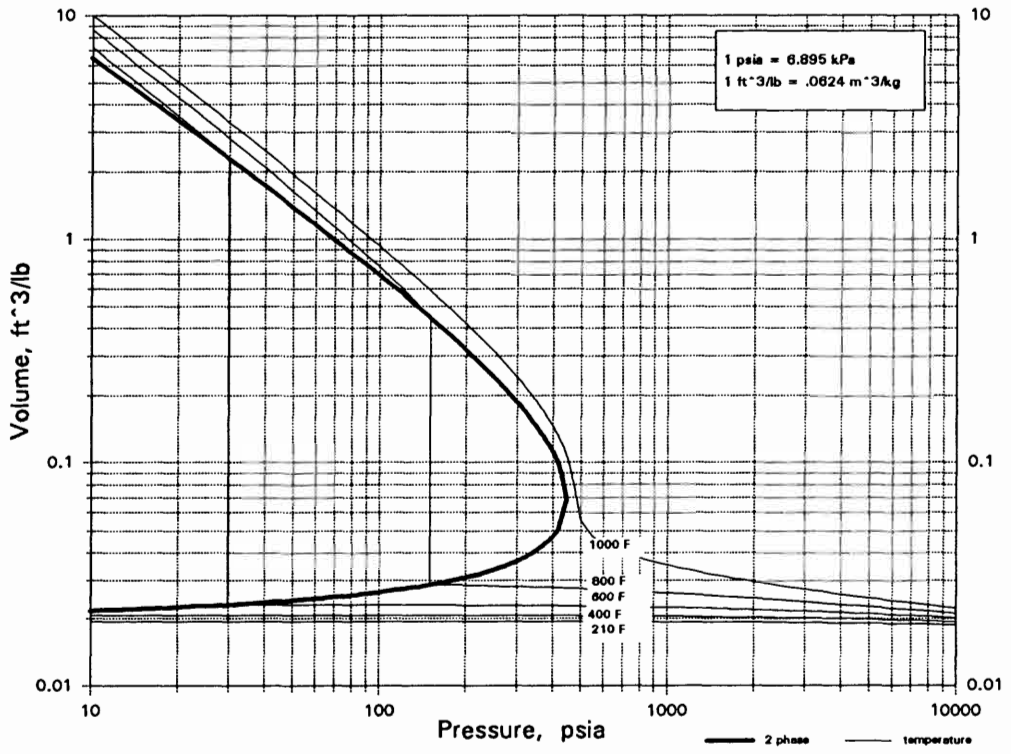


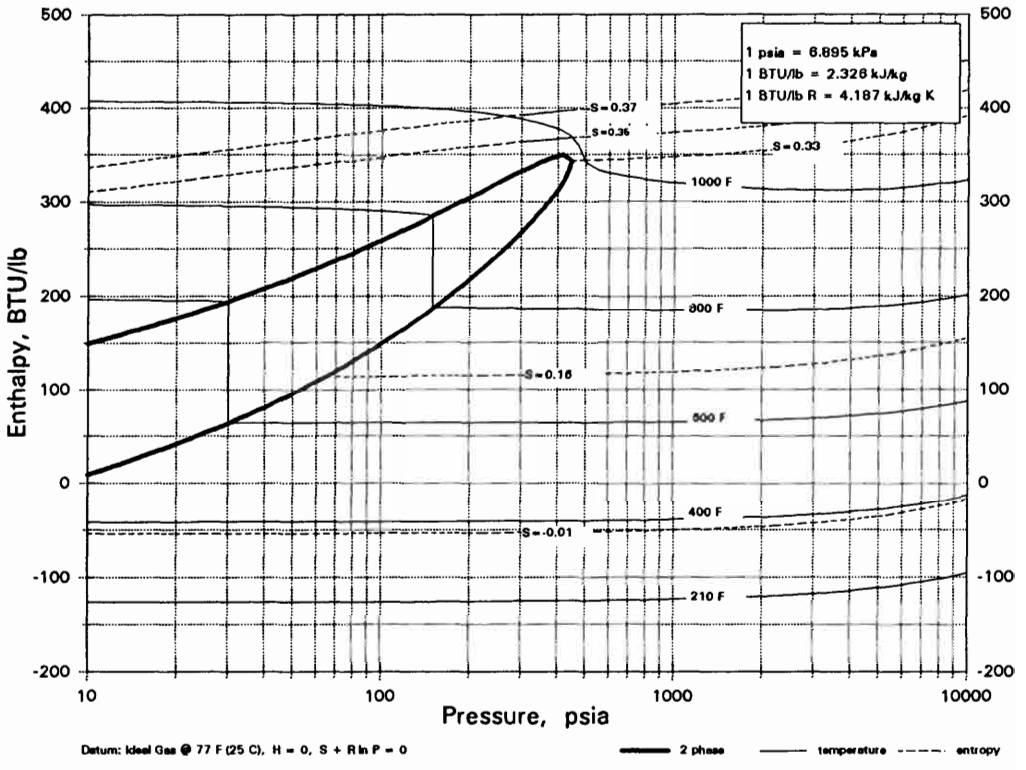
C12H9N DIBENZOPYRROLE



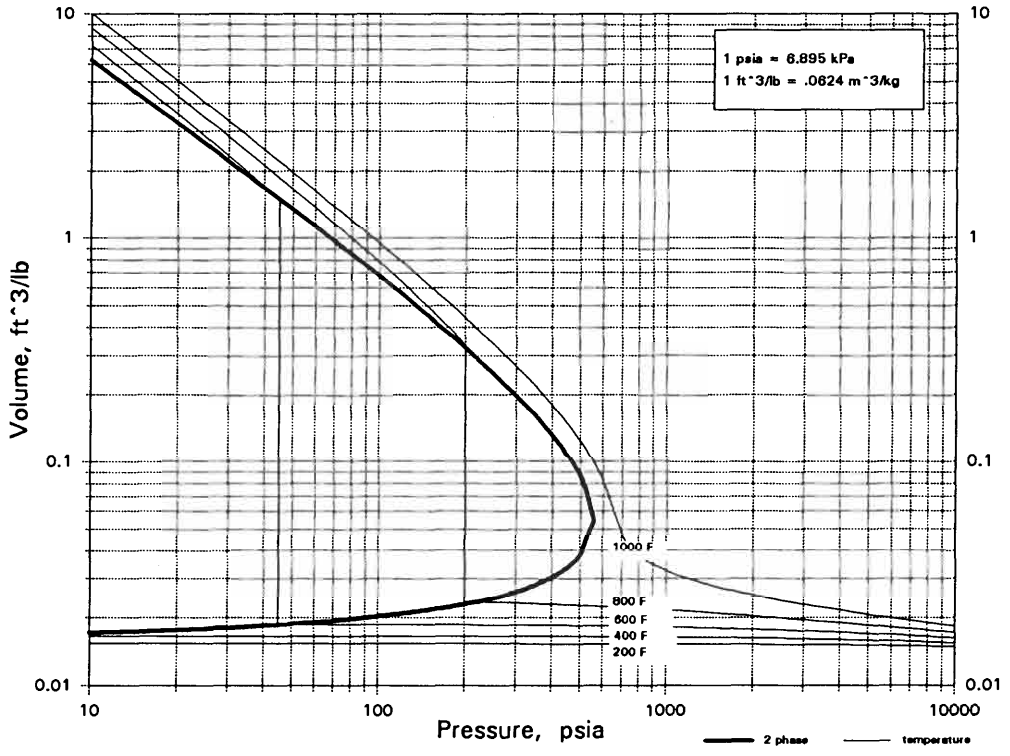


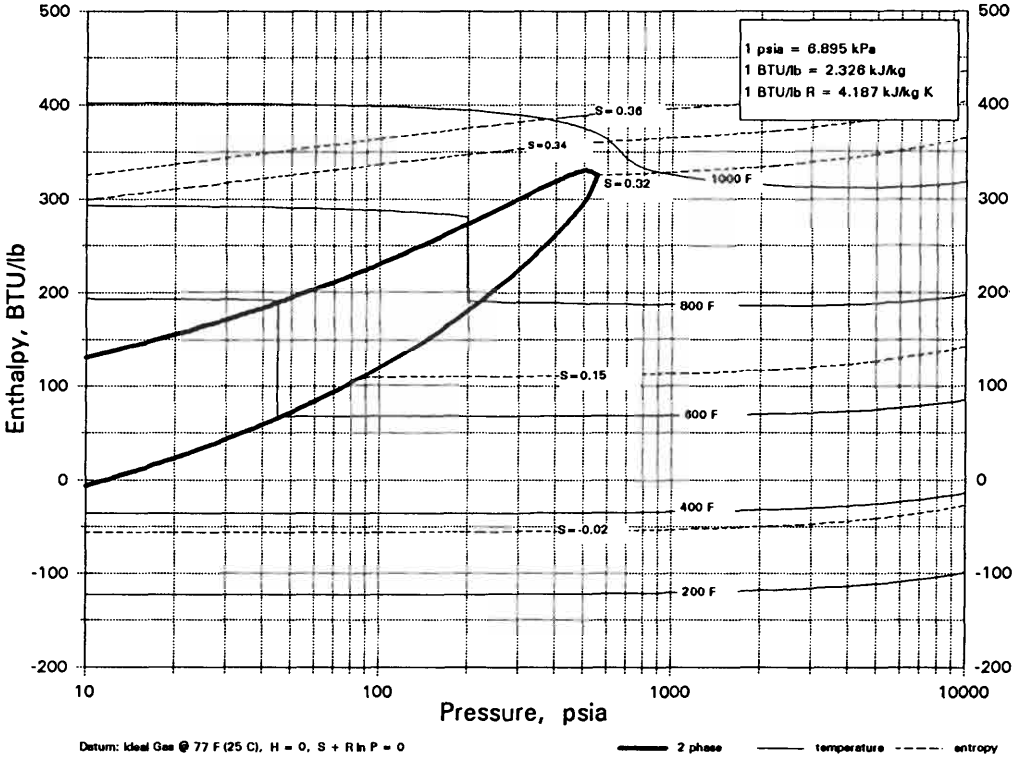
C12H10 ACENAPHTHENE



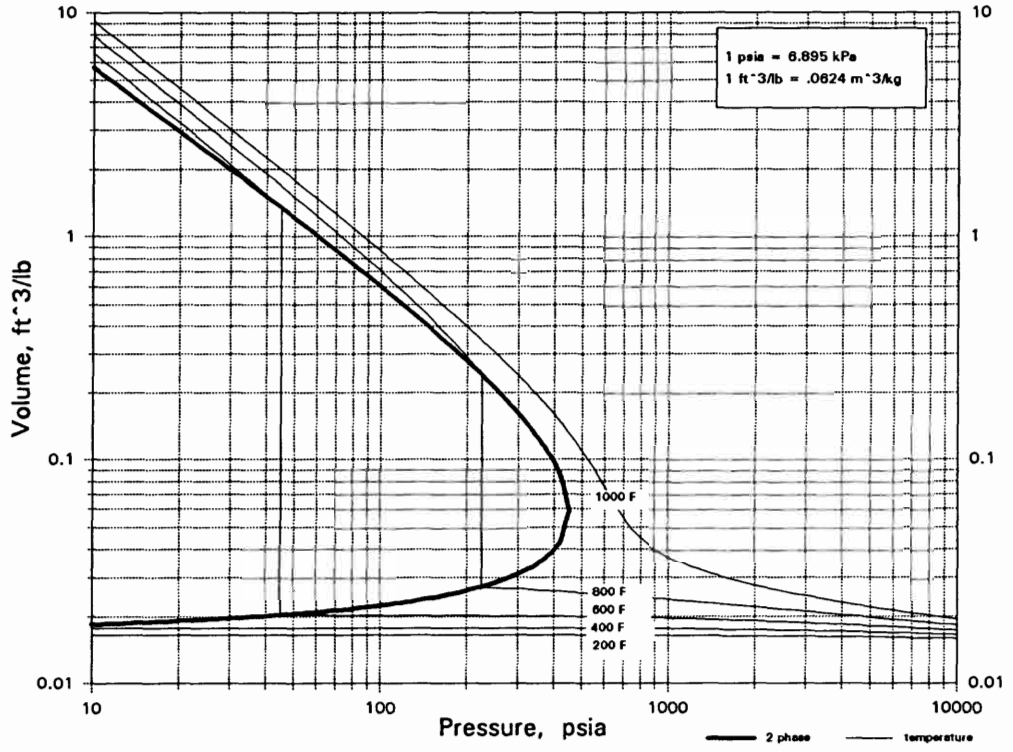


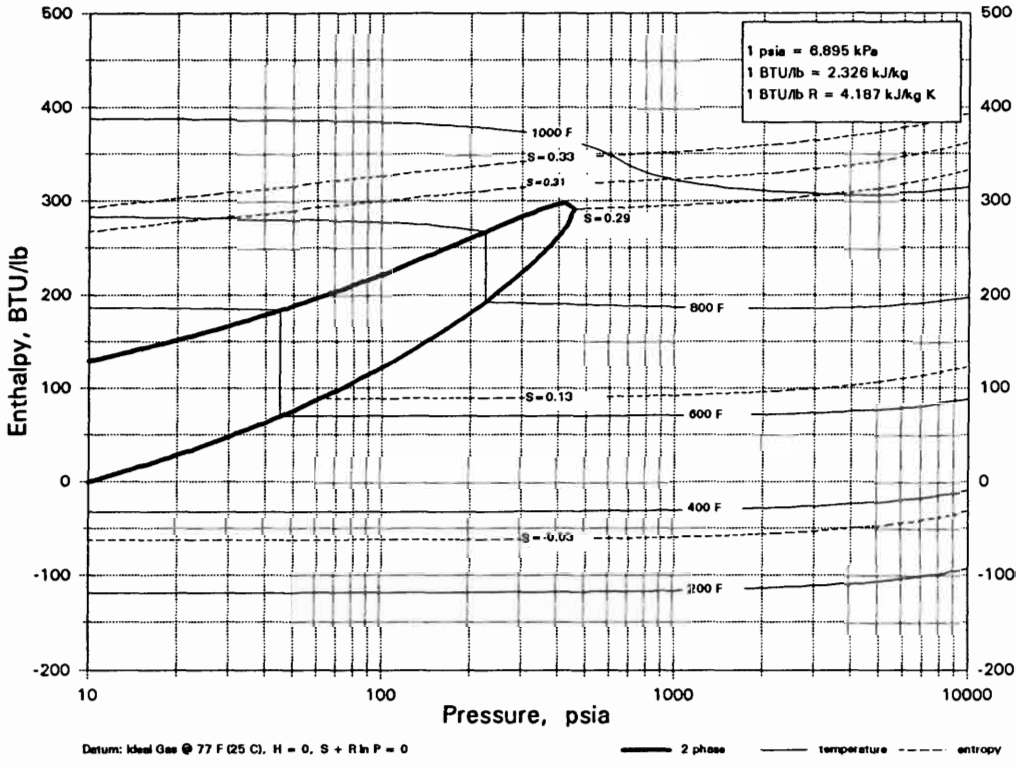
C12H10 BIPHENYL



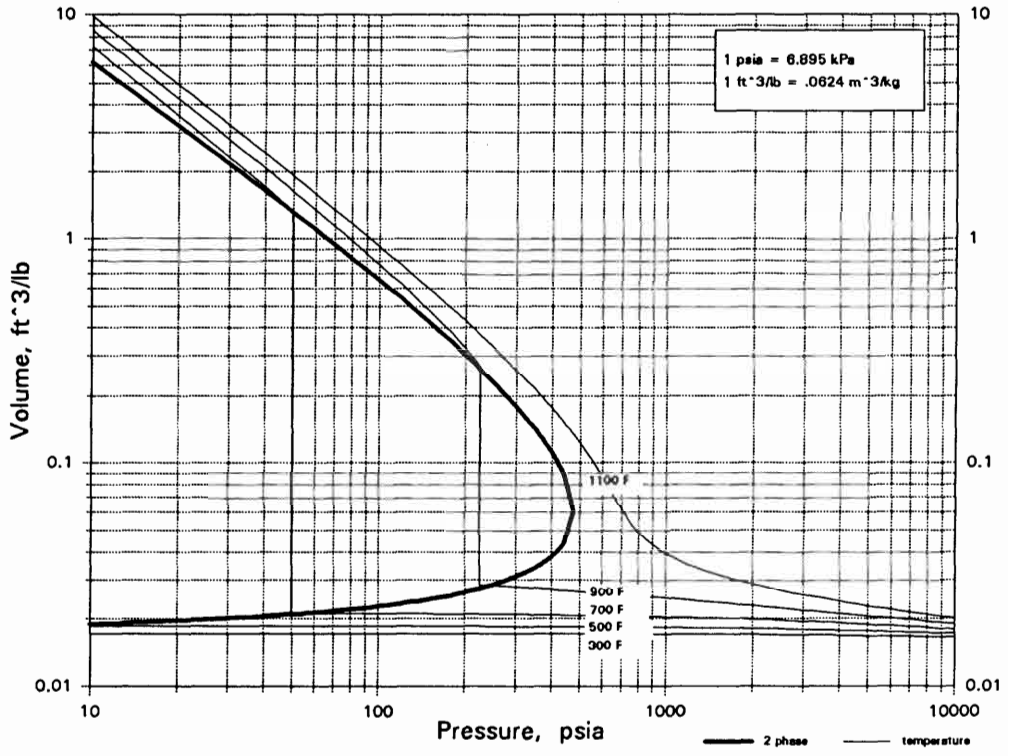


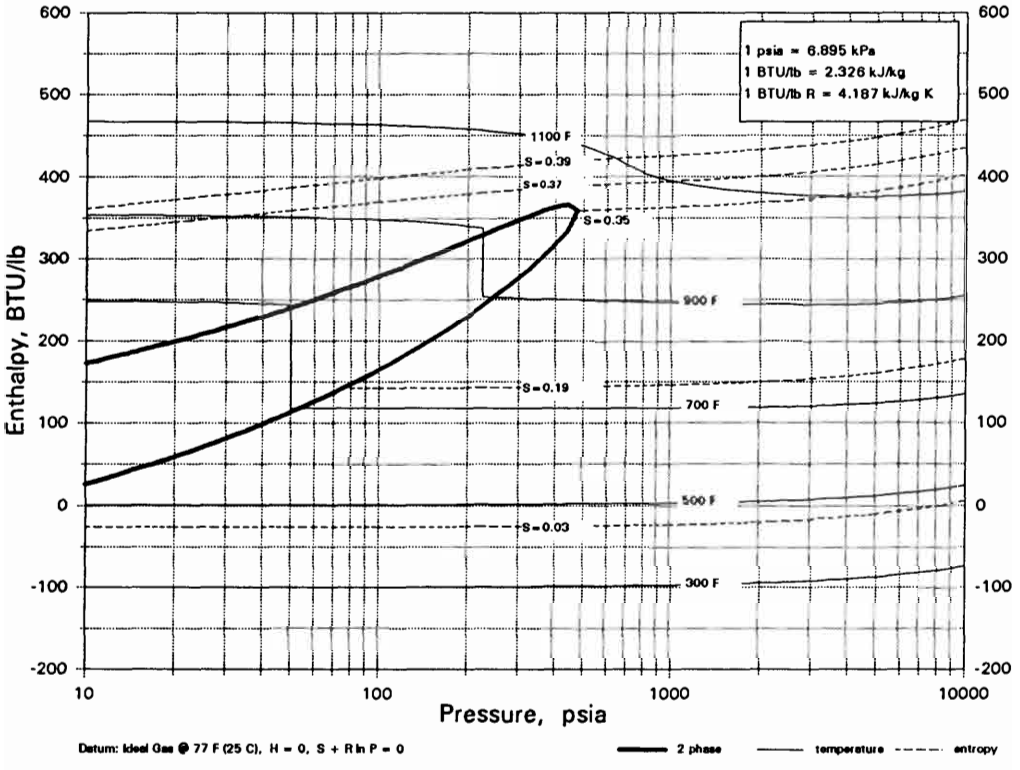
C12H10O DIPHENYL ETHER



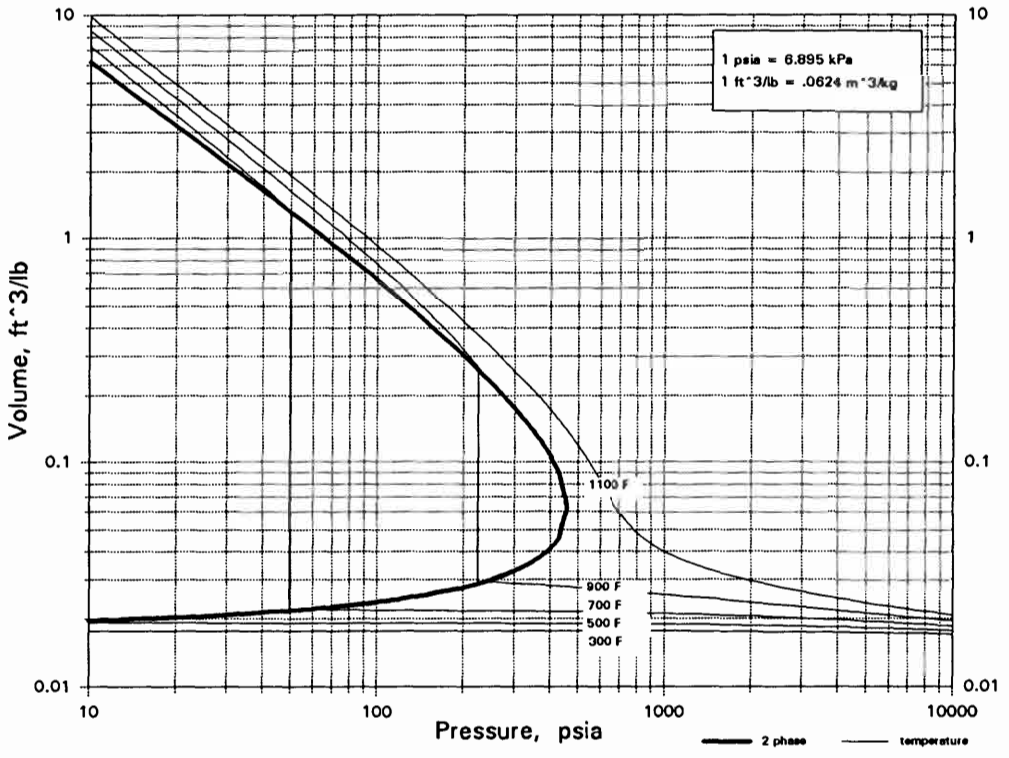


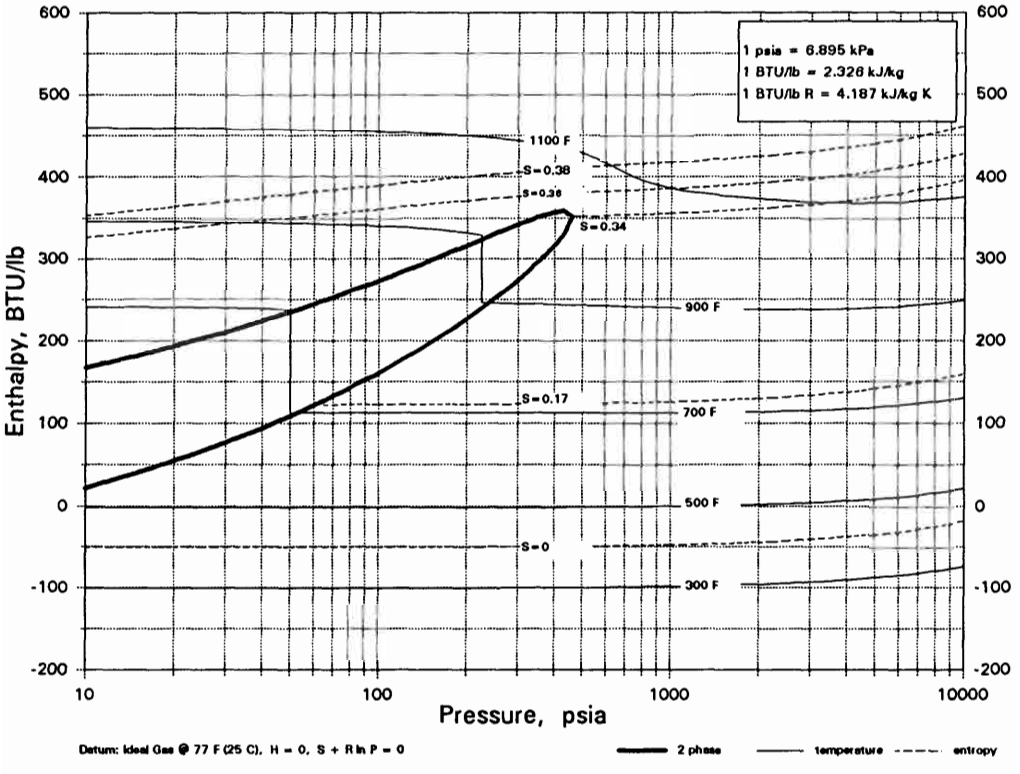
C12H11N p-AMINODIPHENYL



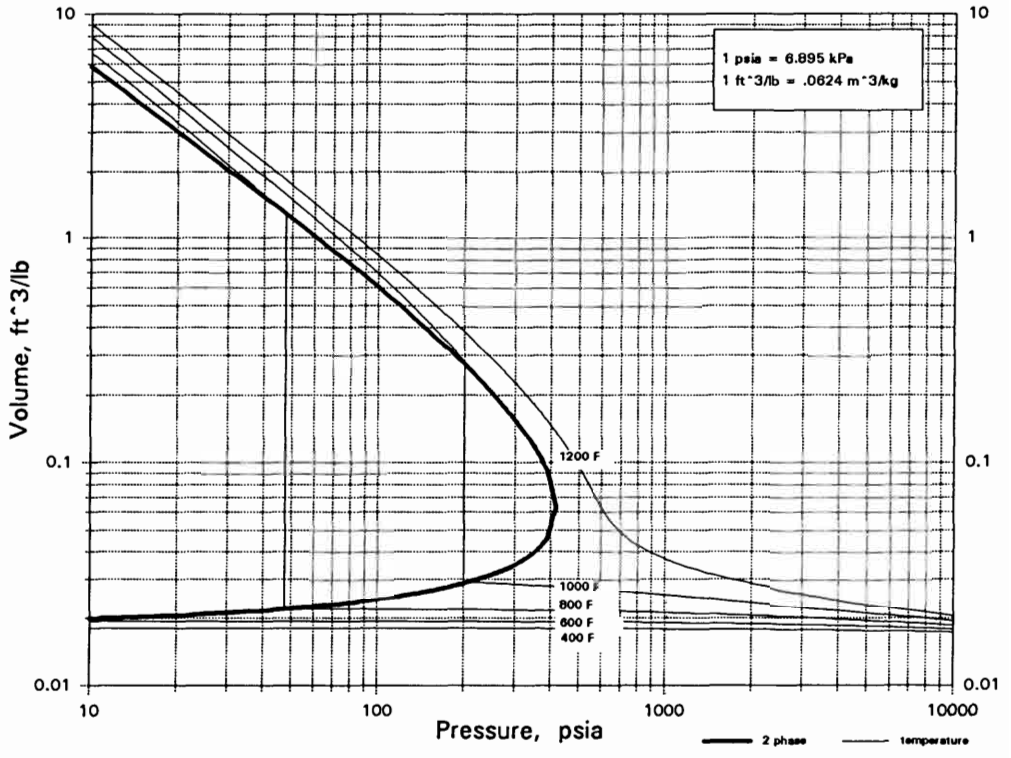


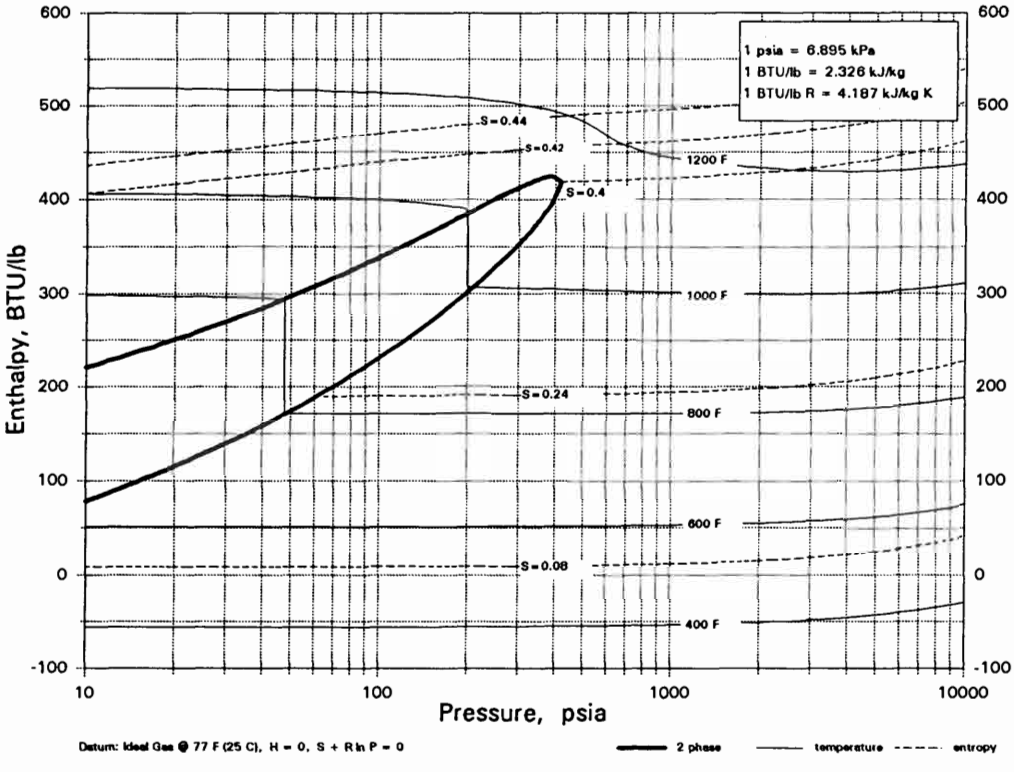
C12H11N DIPHENYLAMINE



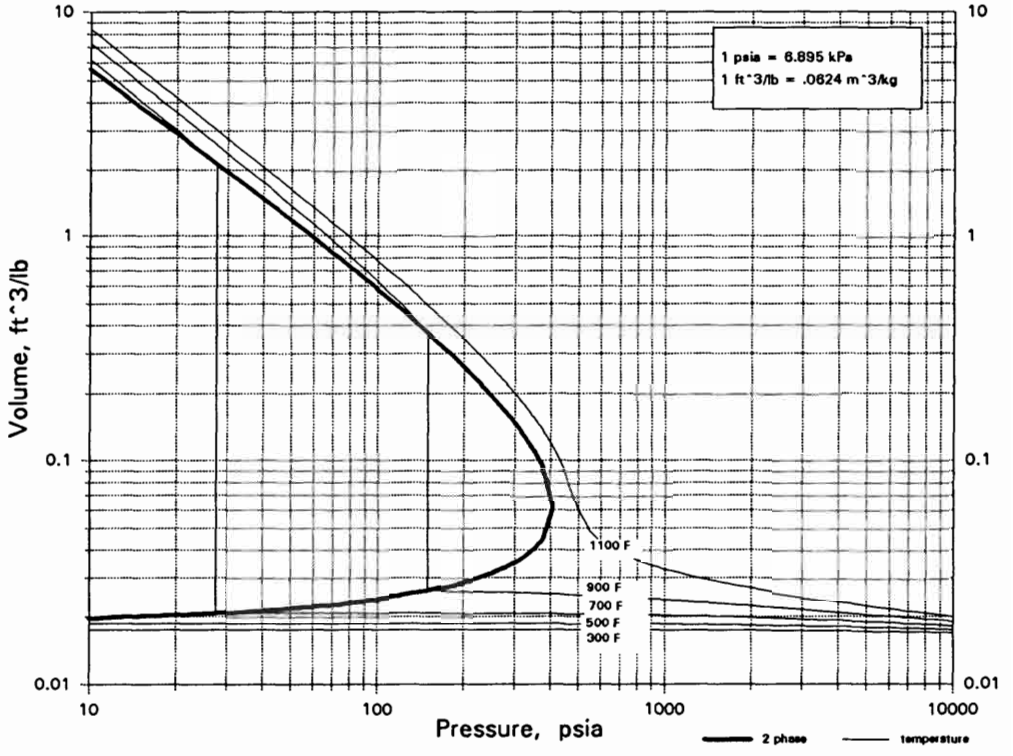


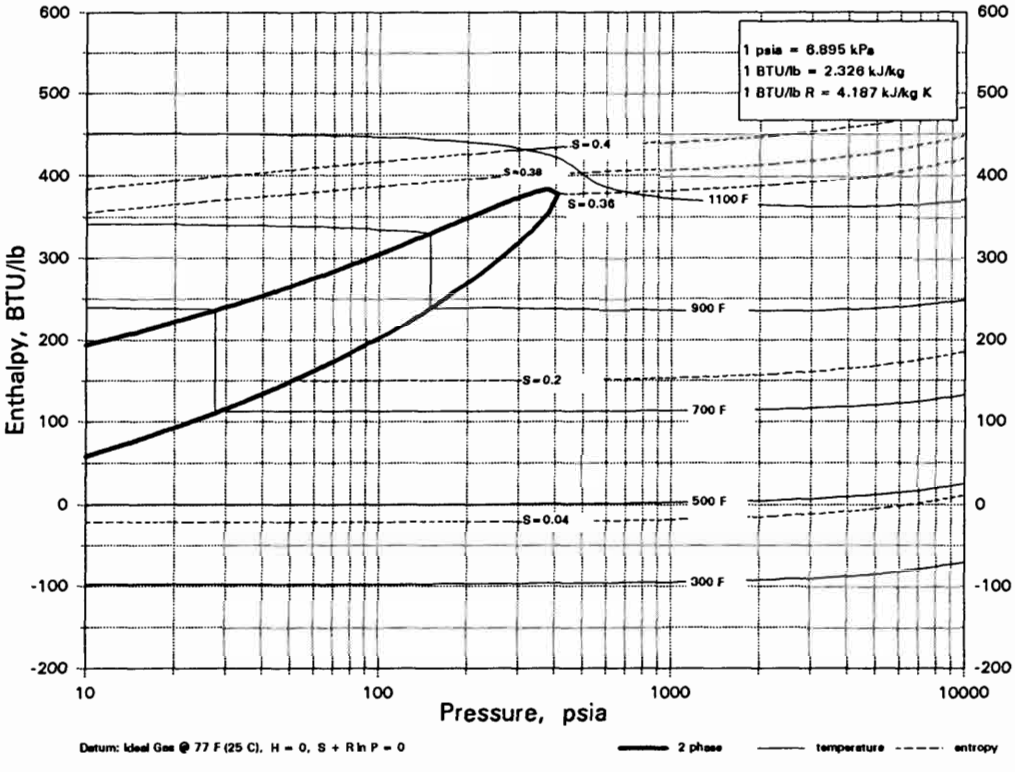
C12H11N3 p-AMINOAZOBENZENE



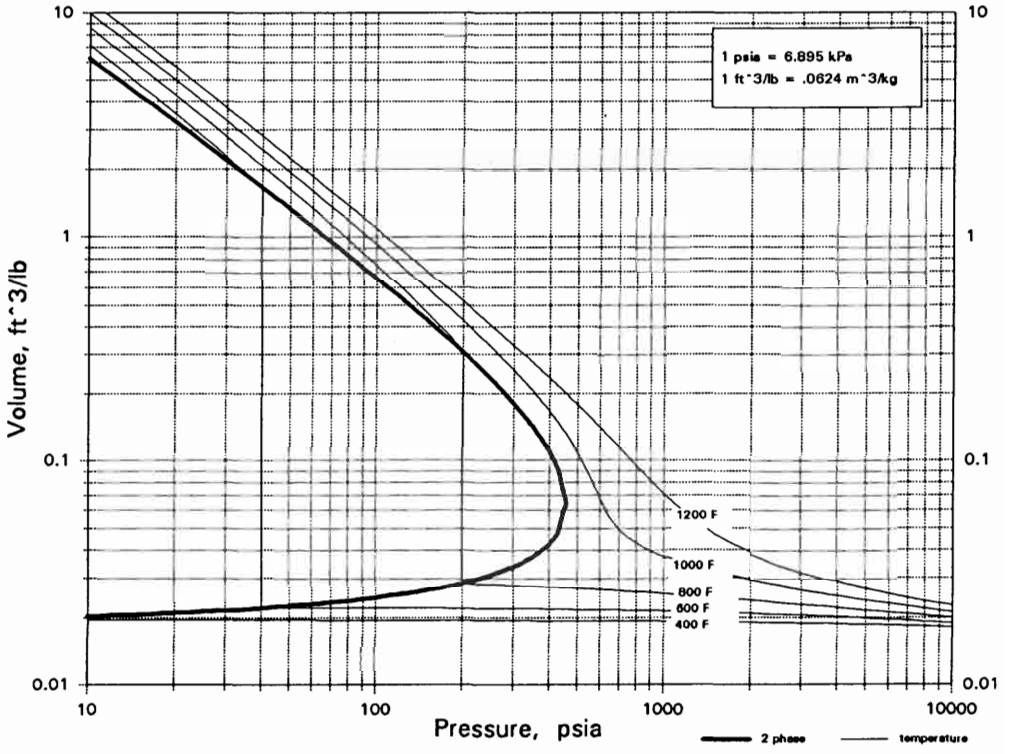


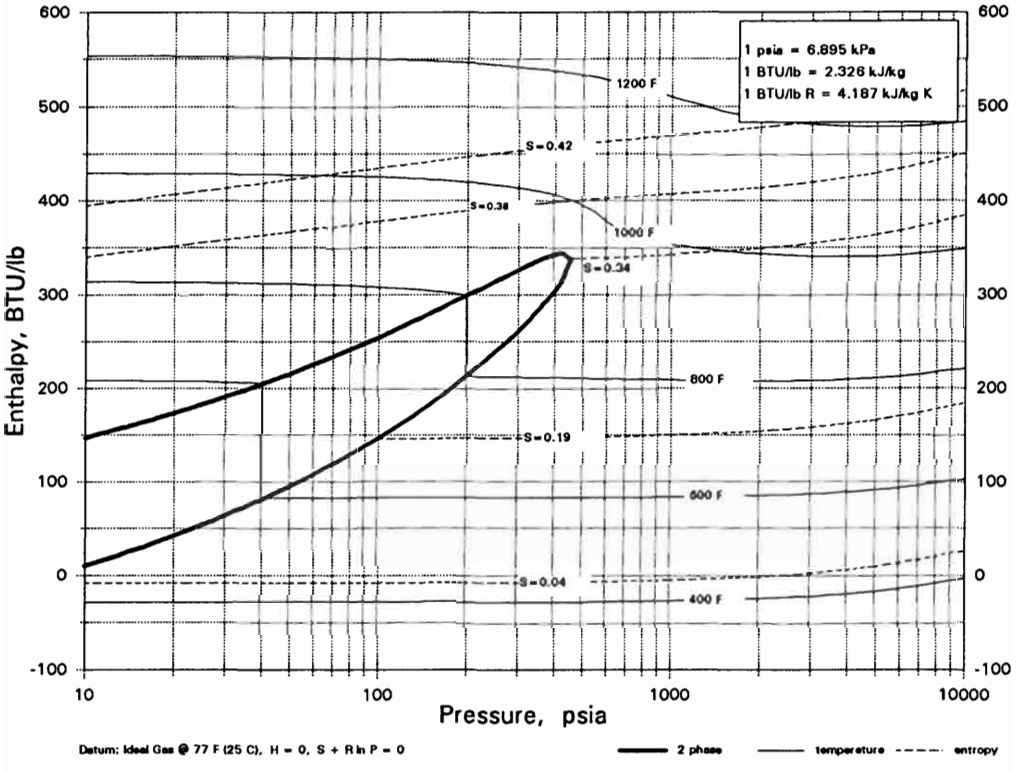
C12H11N3 1-3-DIPHENYLTRIAZENE



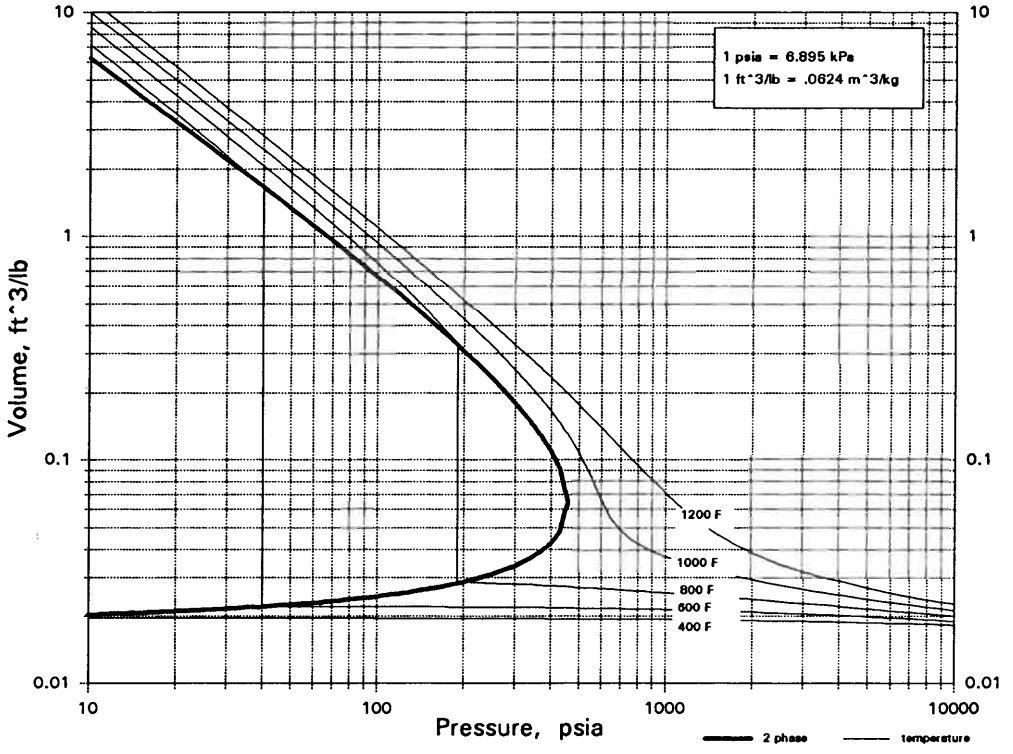


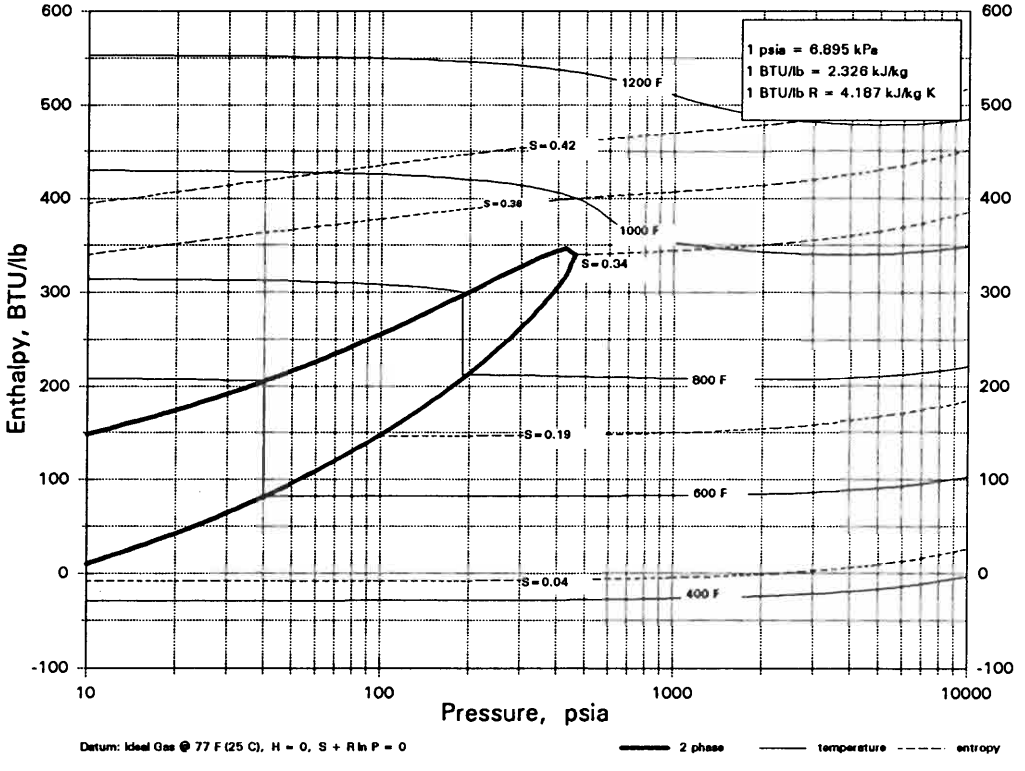
C12H12 2-6-DIMETHYLNAPHTHALENE



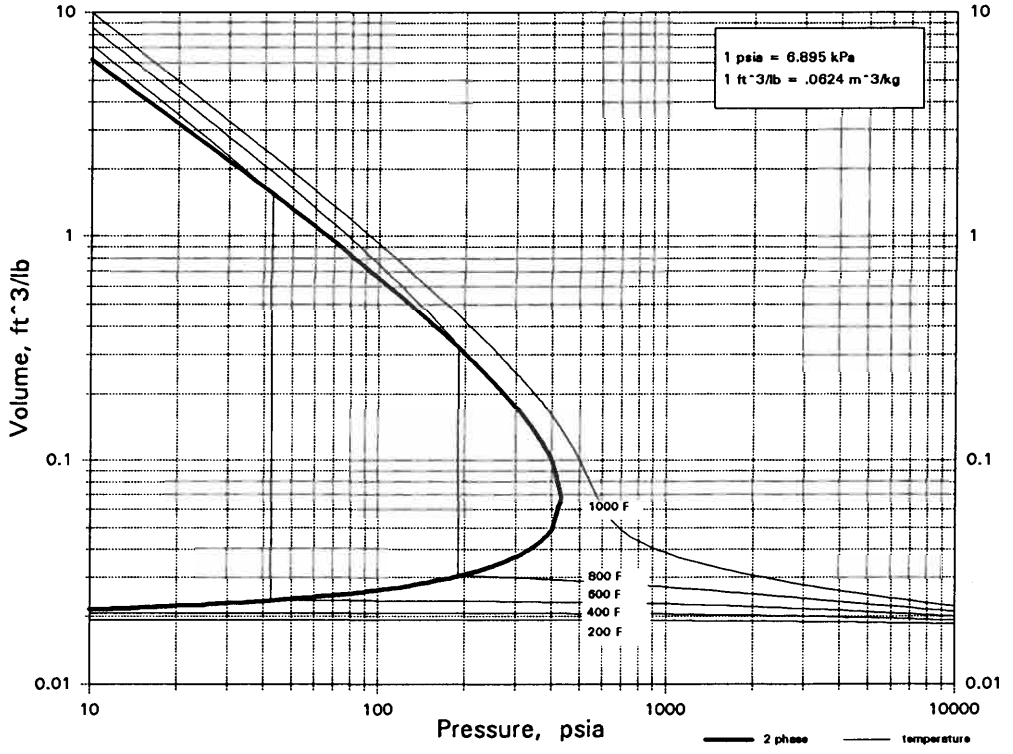


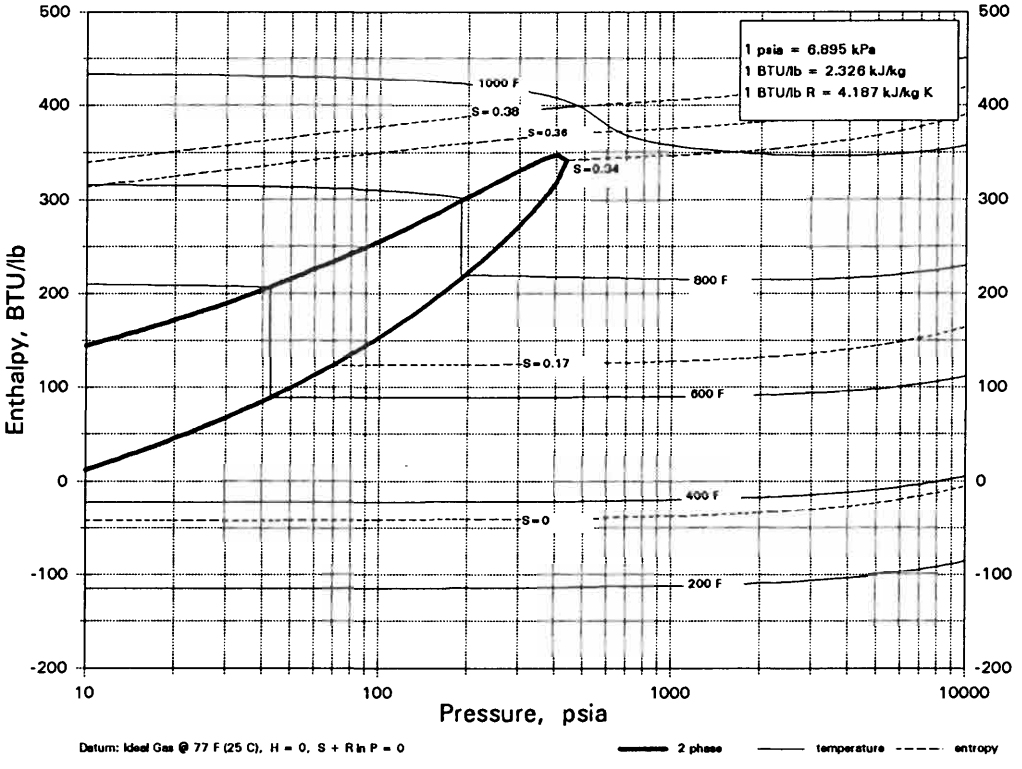
C12H12 2-7-DIMETHYLNAPHTHALENE



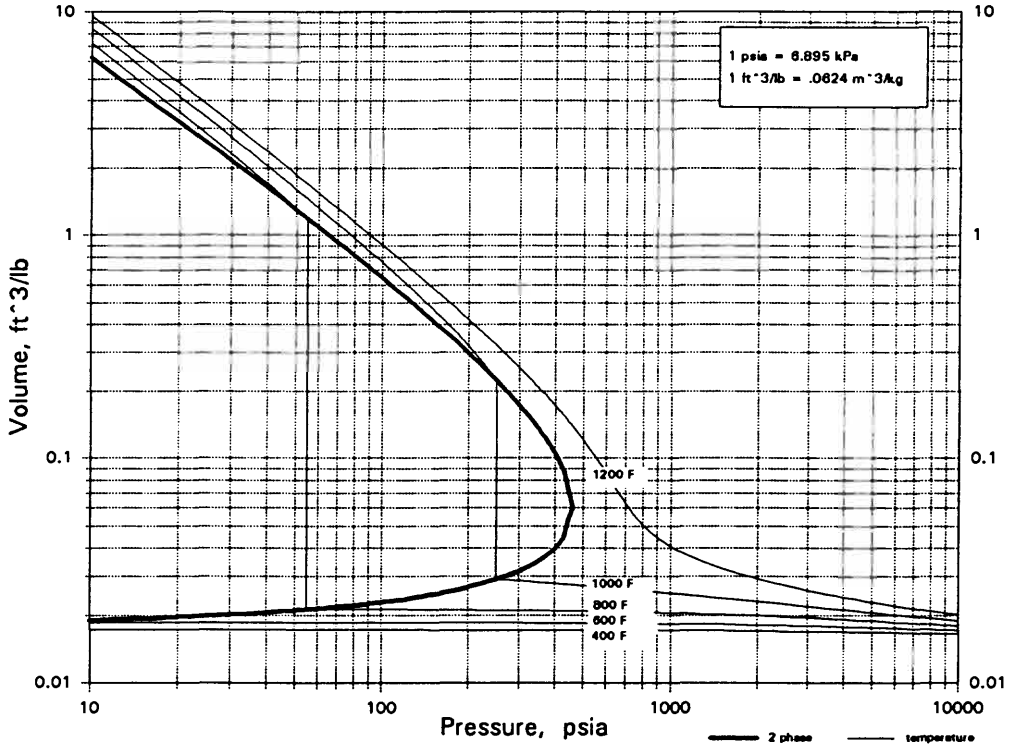


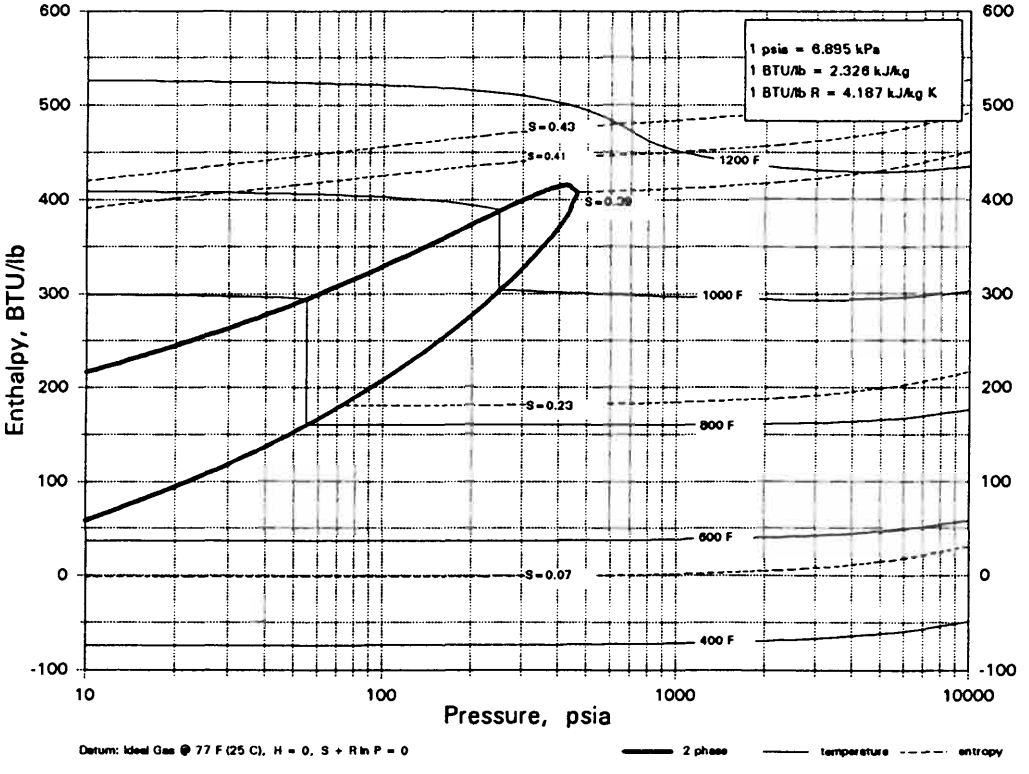
C12H12 1-ETHYLNAPHTHALENE



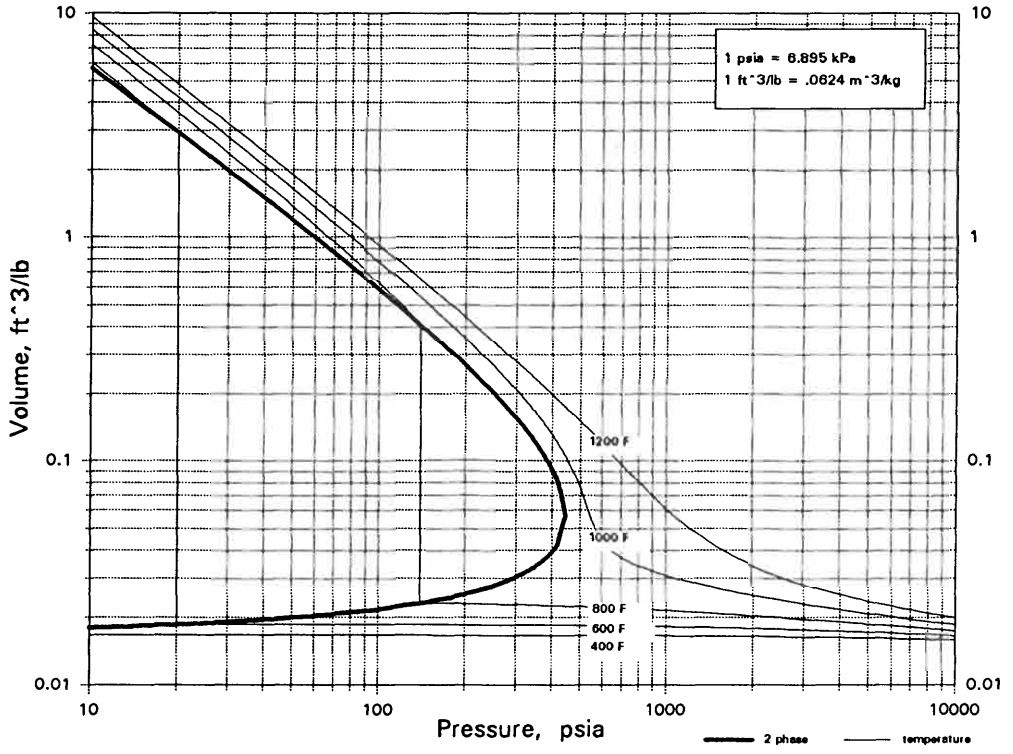


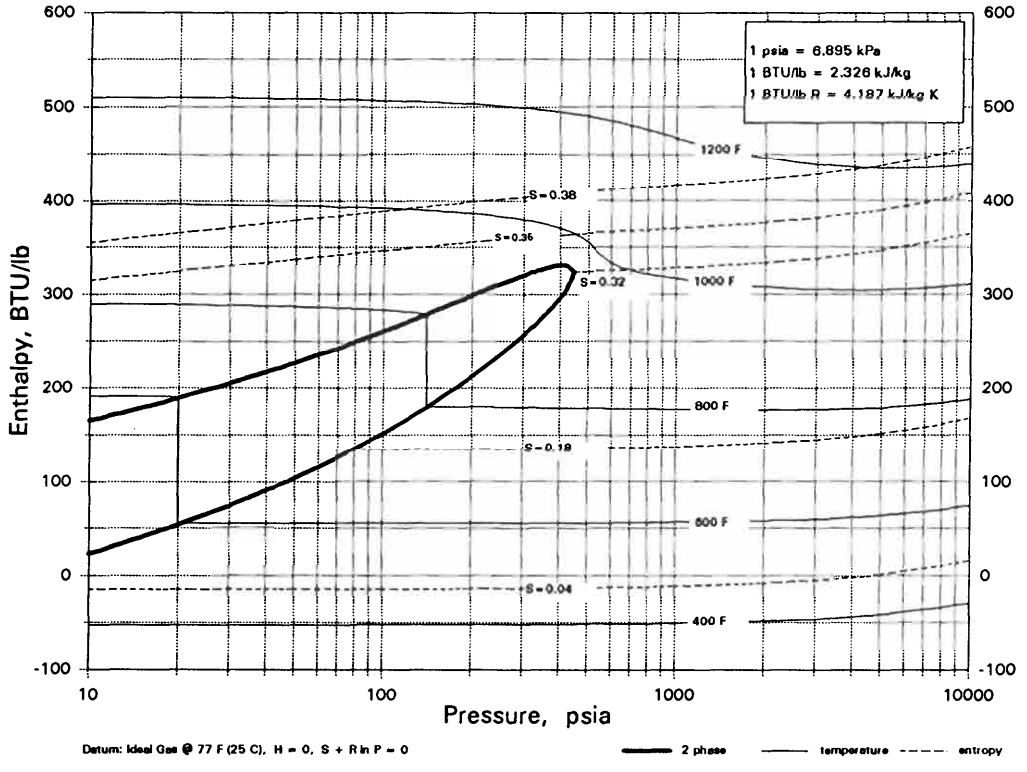
C12H12N2 p-AMINODIPHENYLAMINE



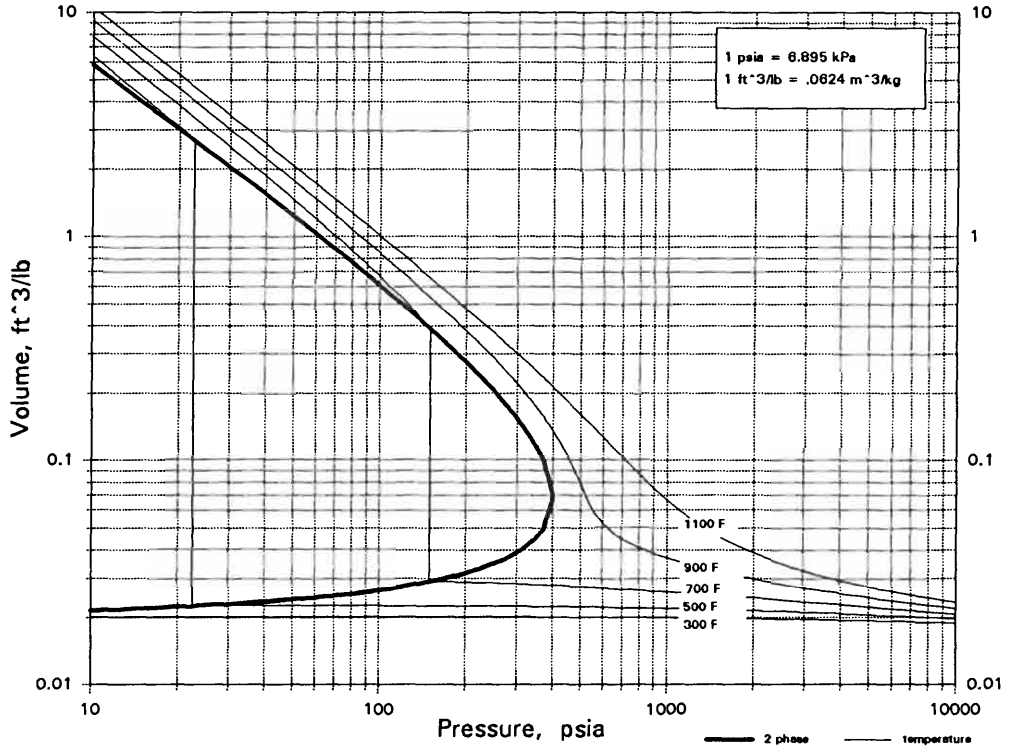


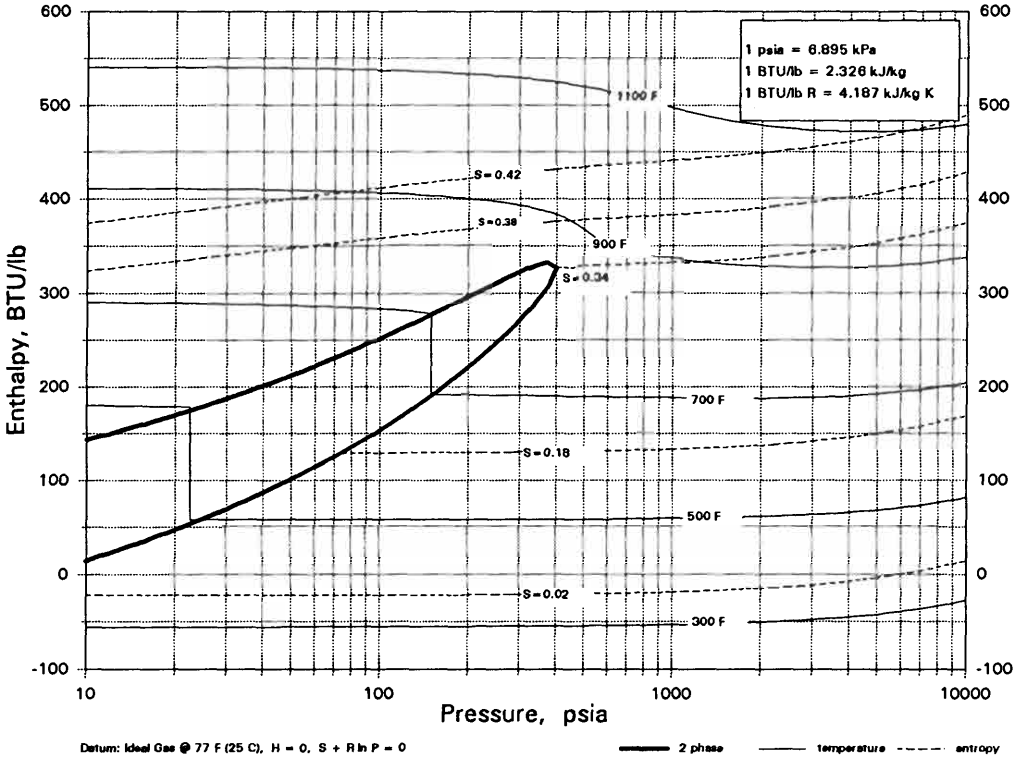
C12H12N2 HYDRAZOBENZENE



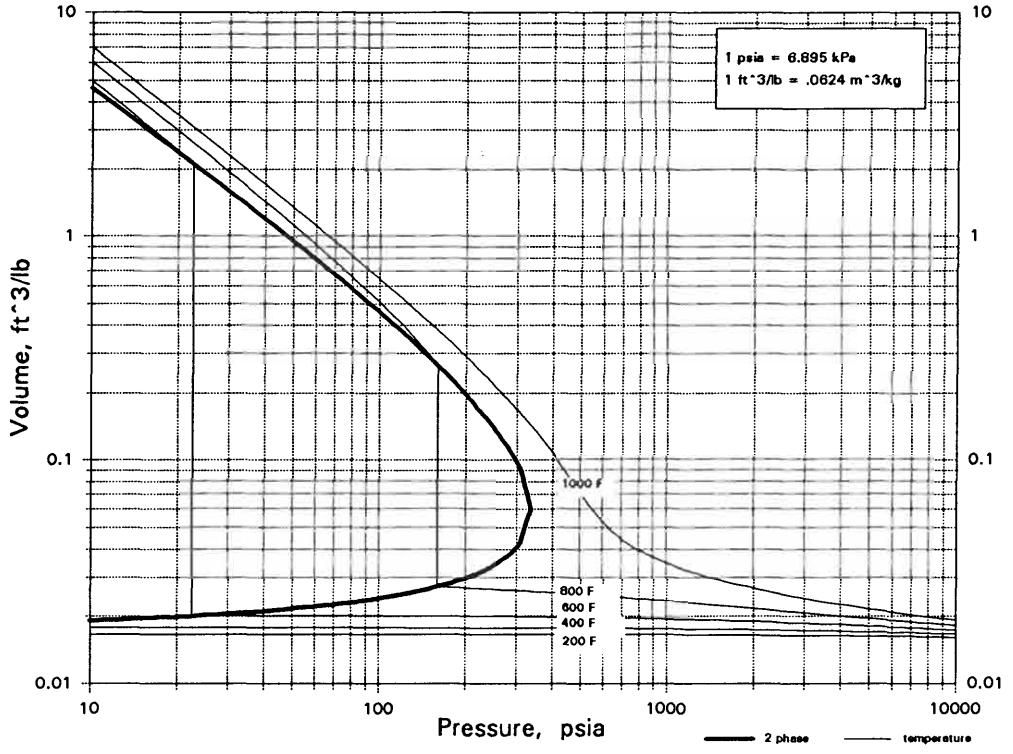


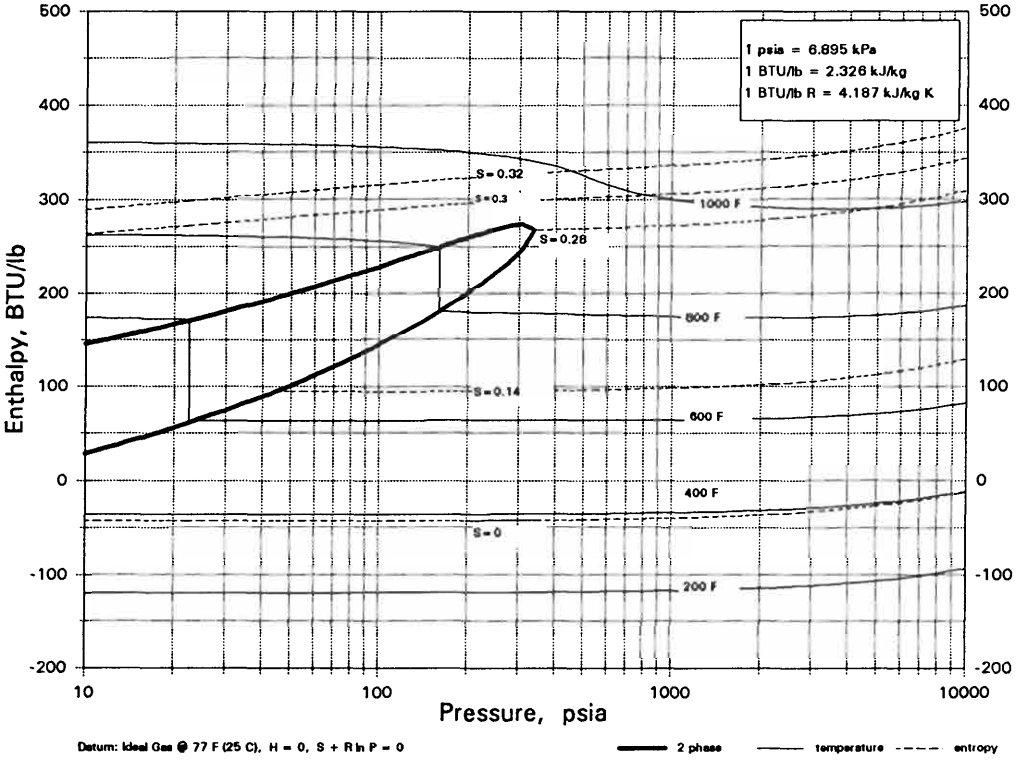
C12H14 1-2-3-TRIMETHYLINDENE



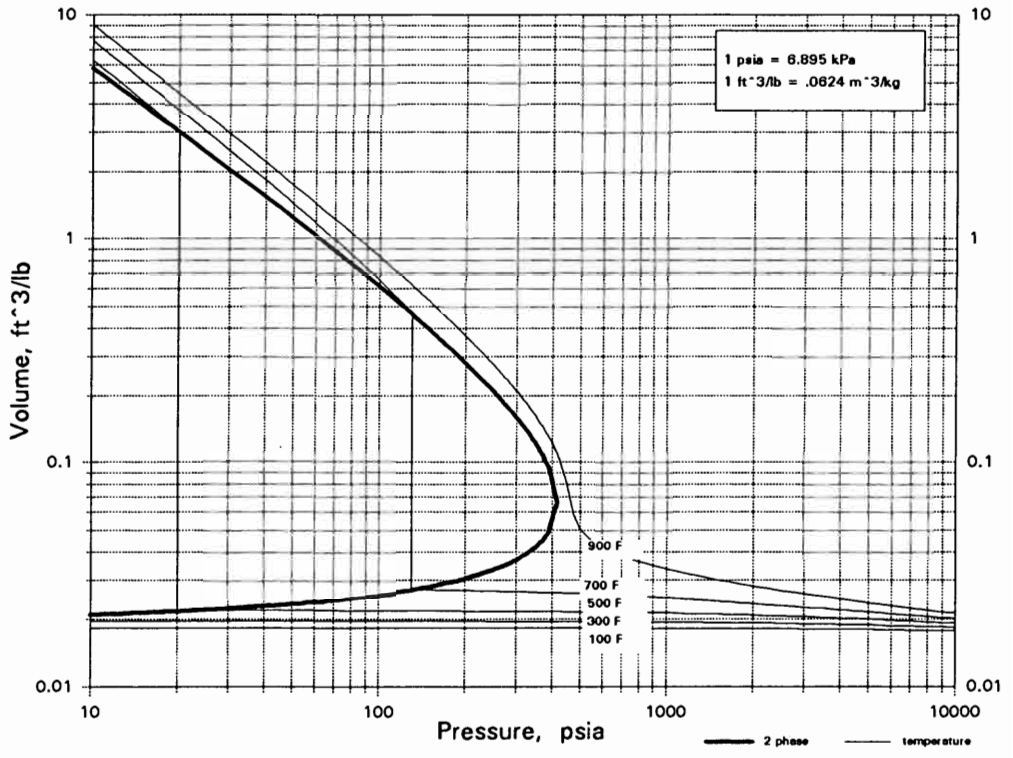


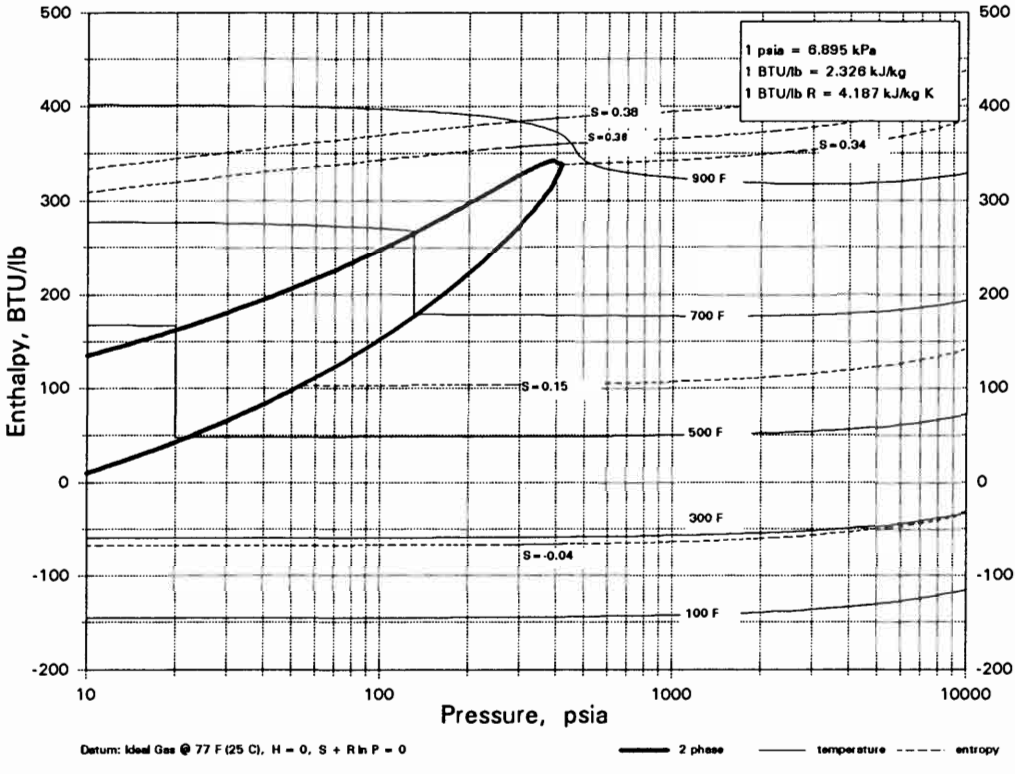
C12H14O4 DIETHYL PHTHALATE



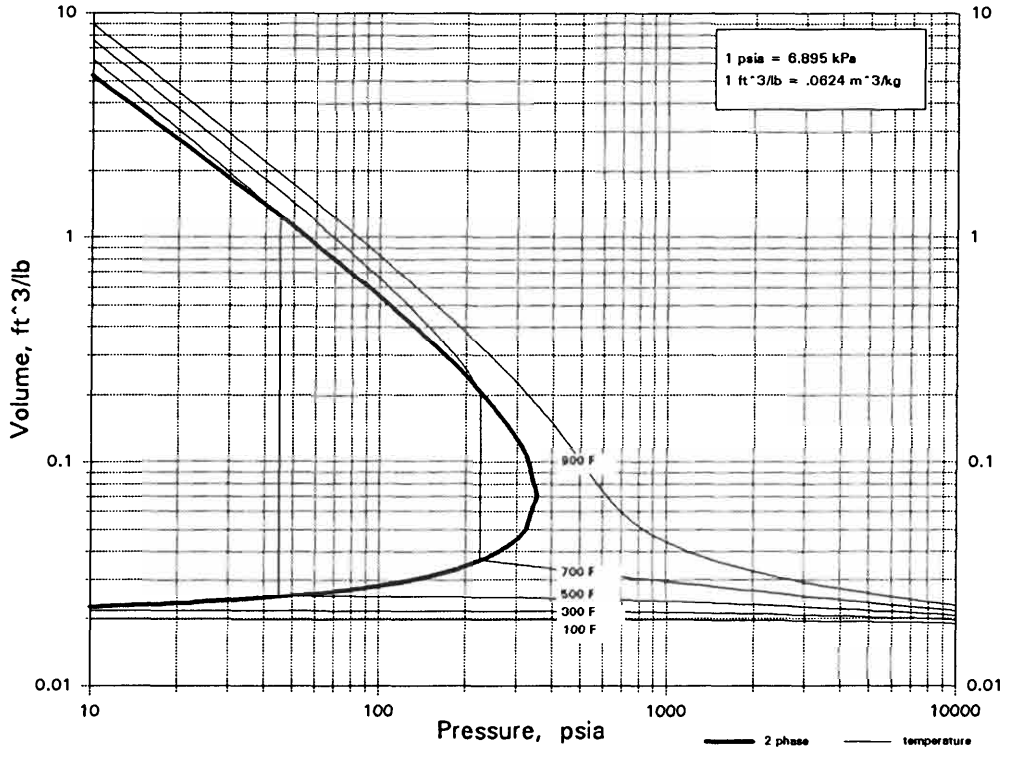


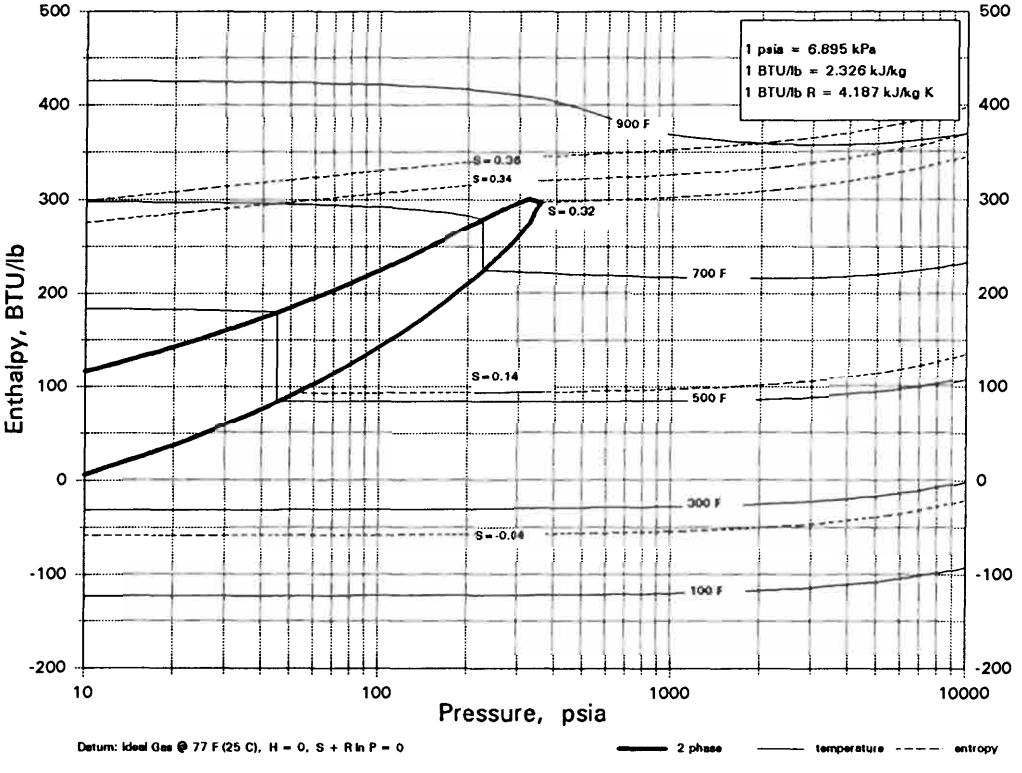
C12H16 CYCLOHEXYLBENZENE



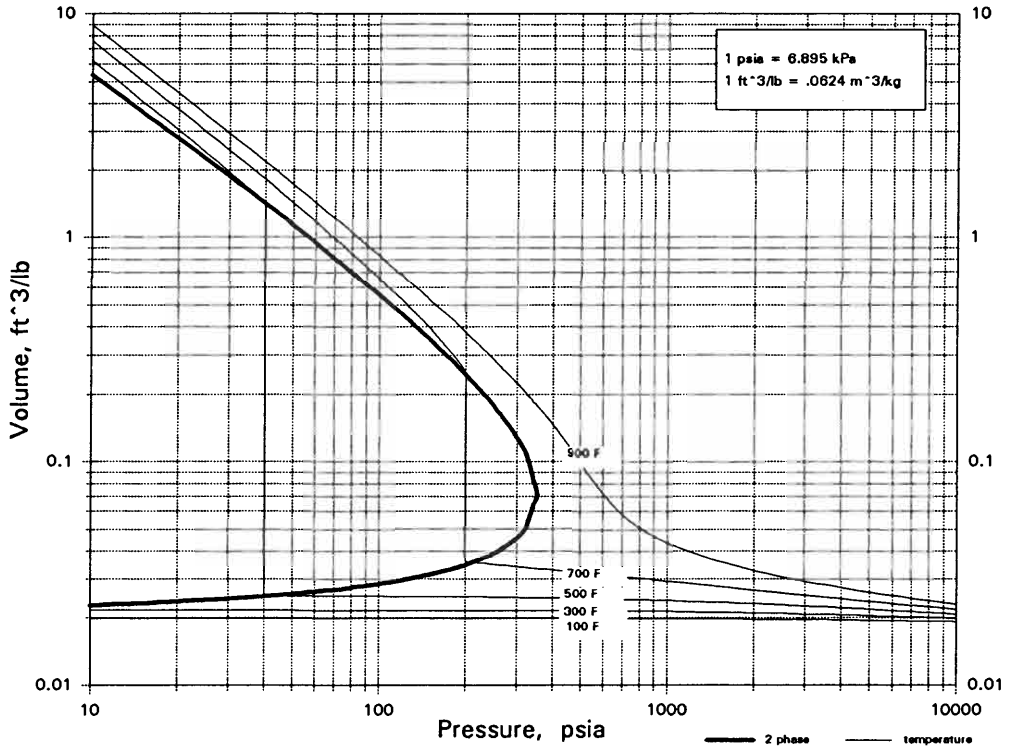


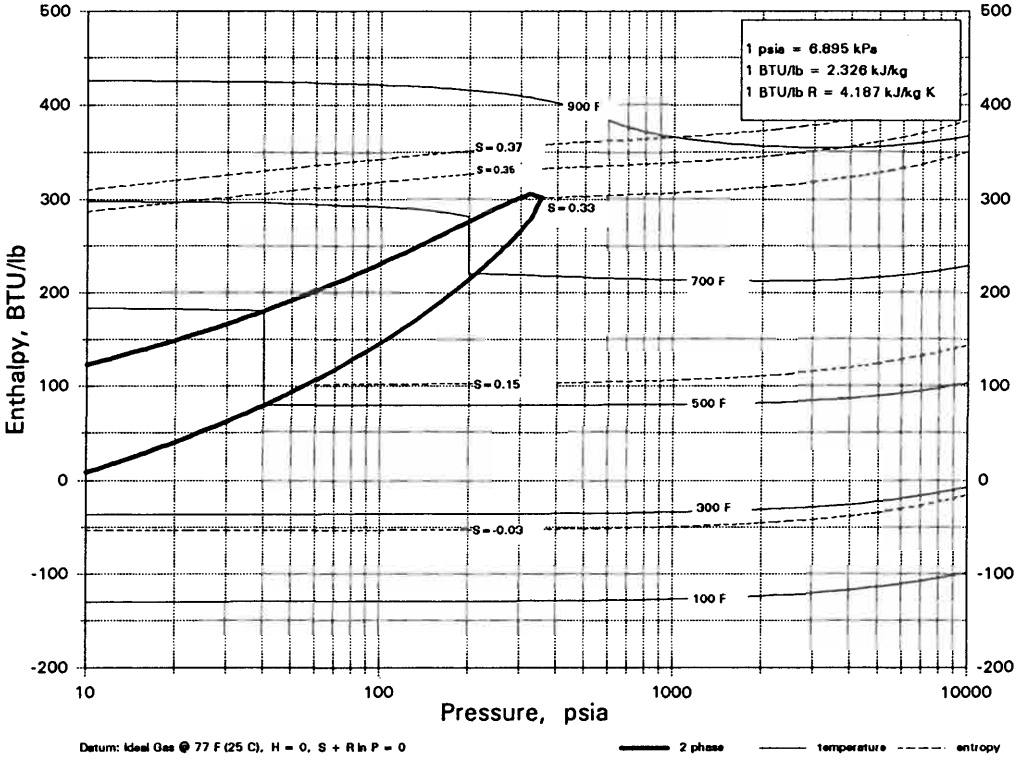
C12H18 m-DIISOPROPYLBENZENE



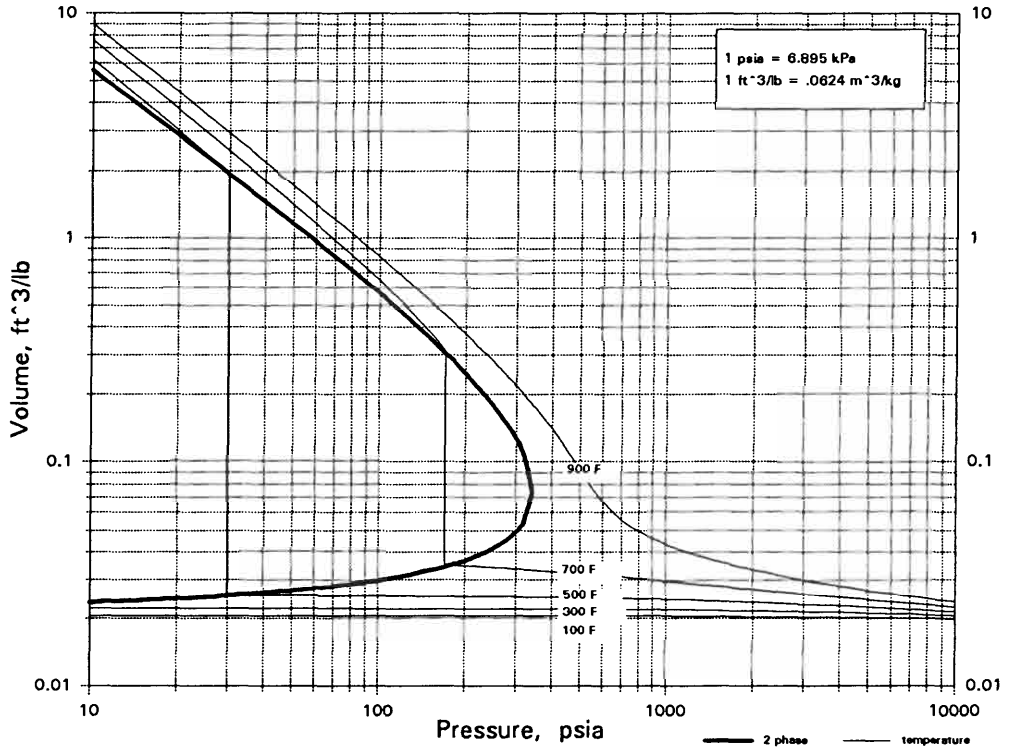


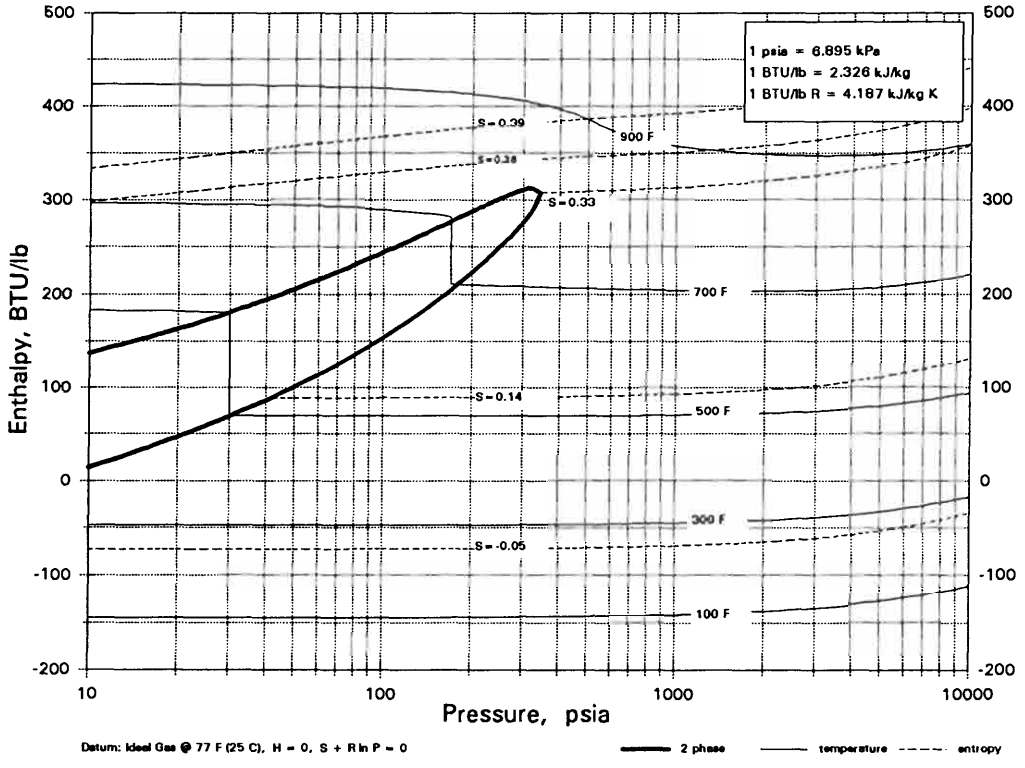
C12H18 p-DIISOPROPYLBENZENE



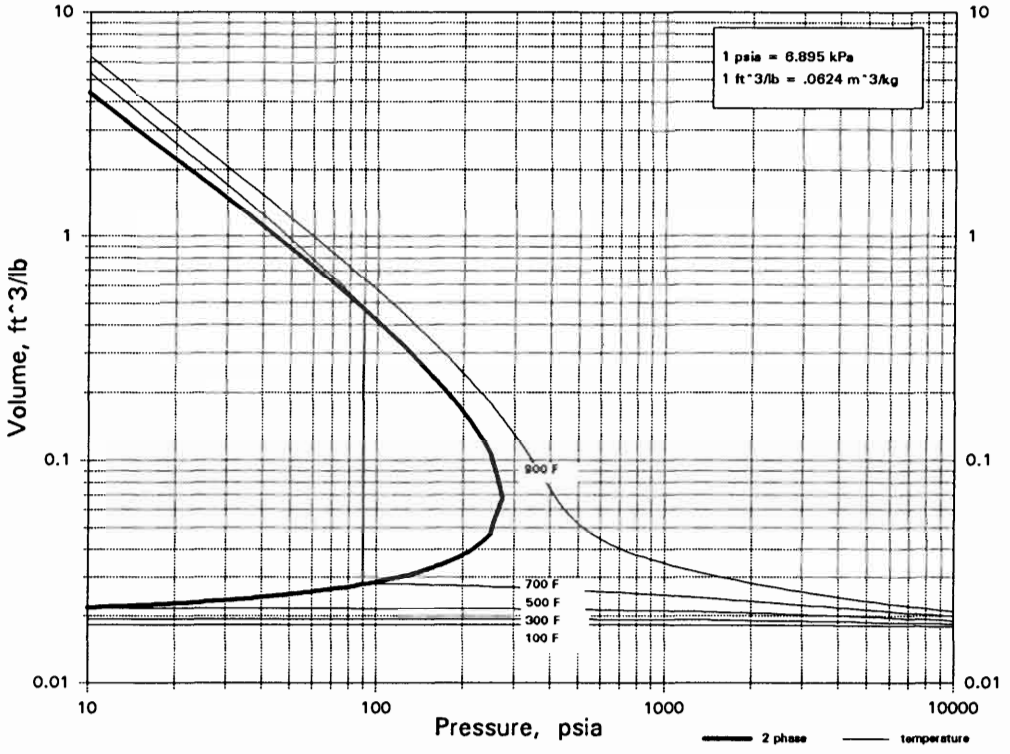


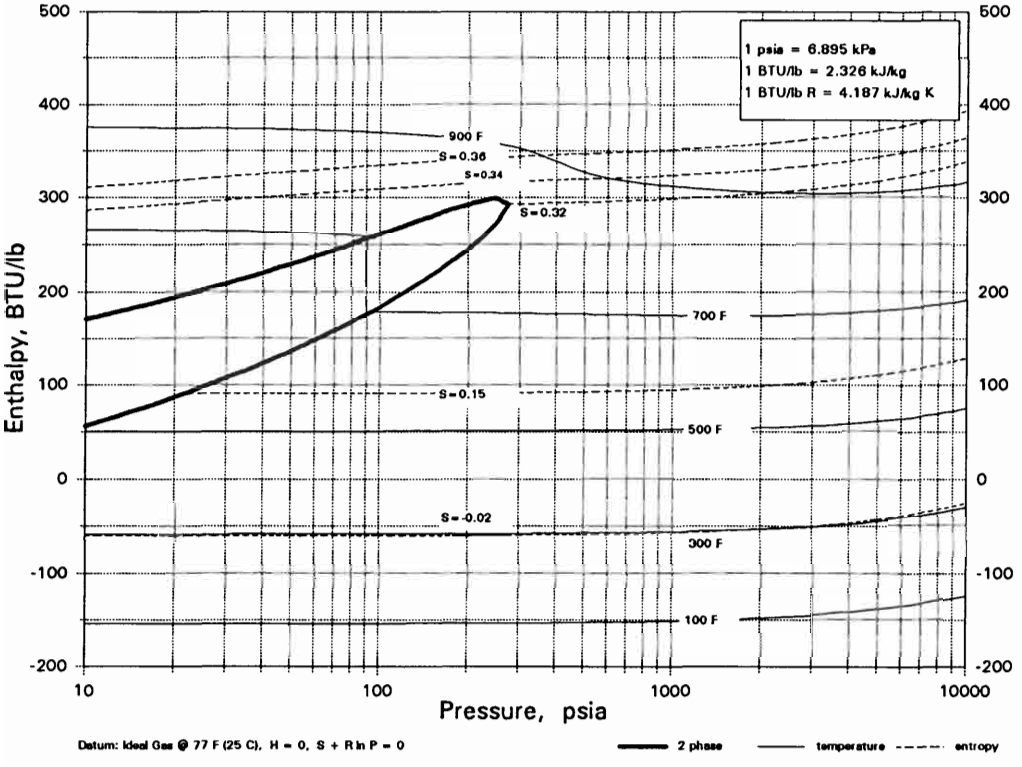
C12H18 n-HEXYLBENZENE



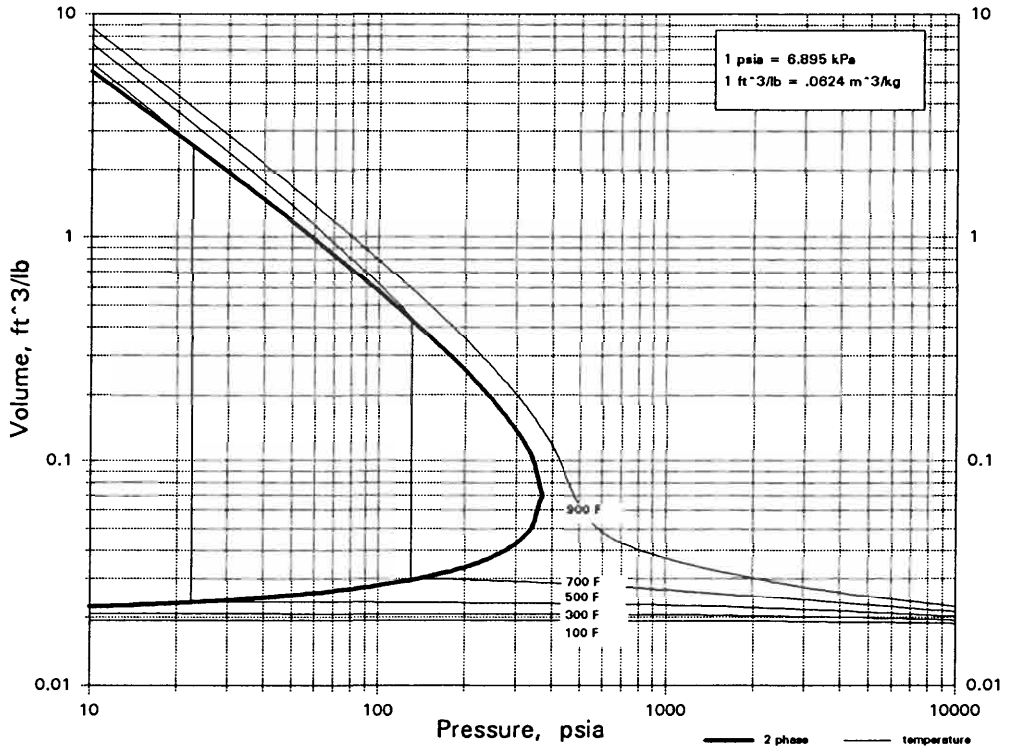


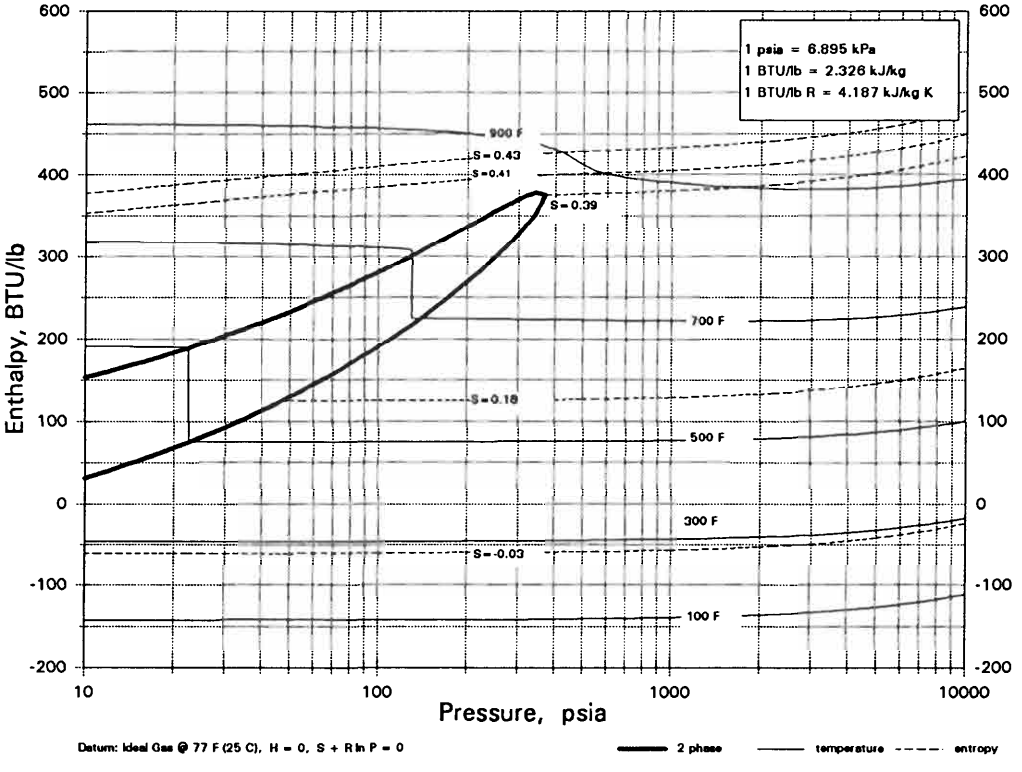
C12H20O4 DIBUTYL MALEATE



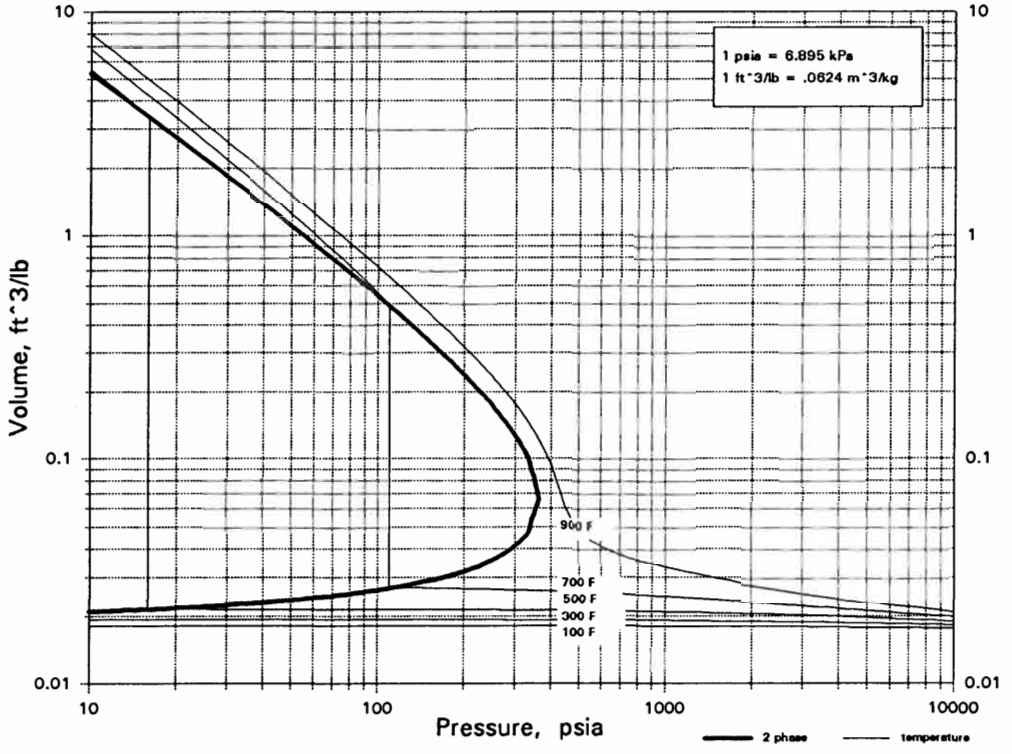


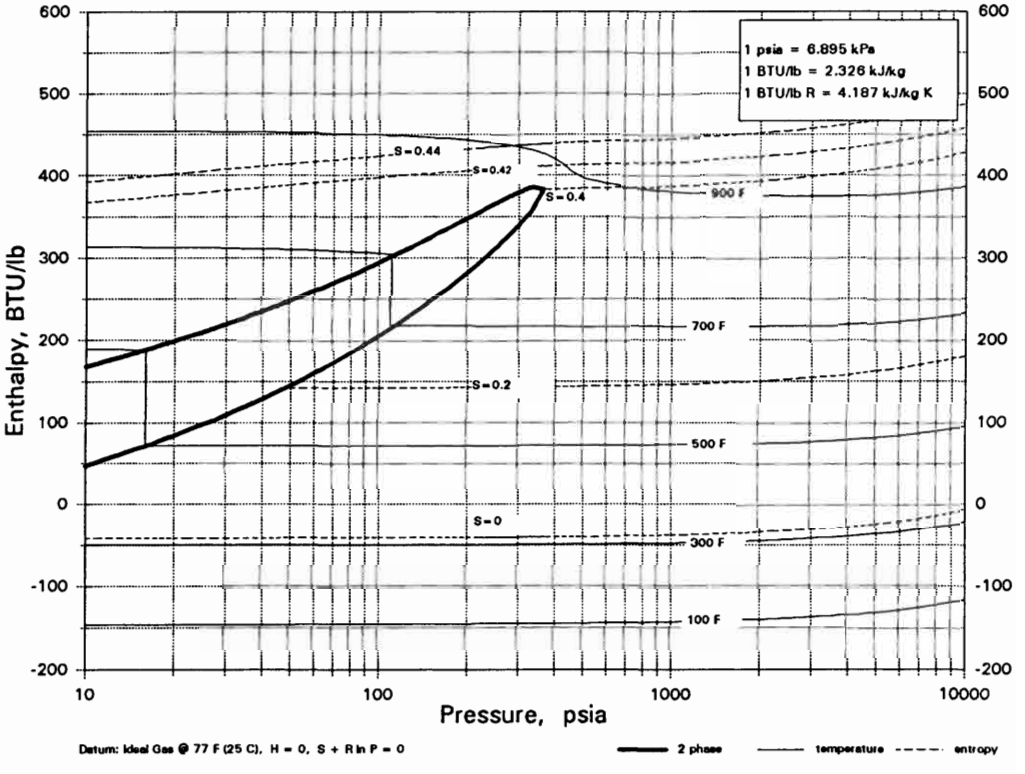
C12H22 BICYCLOHEXYL



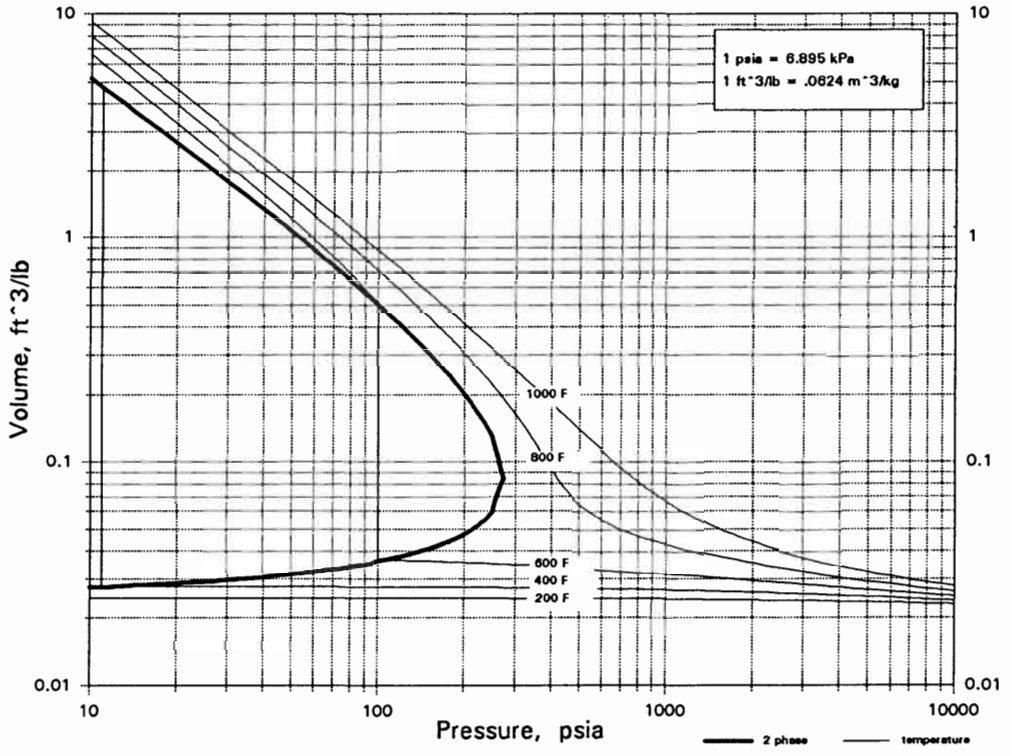


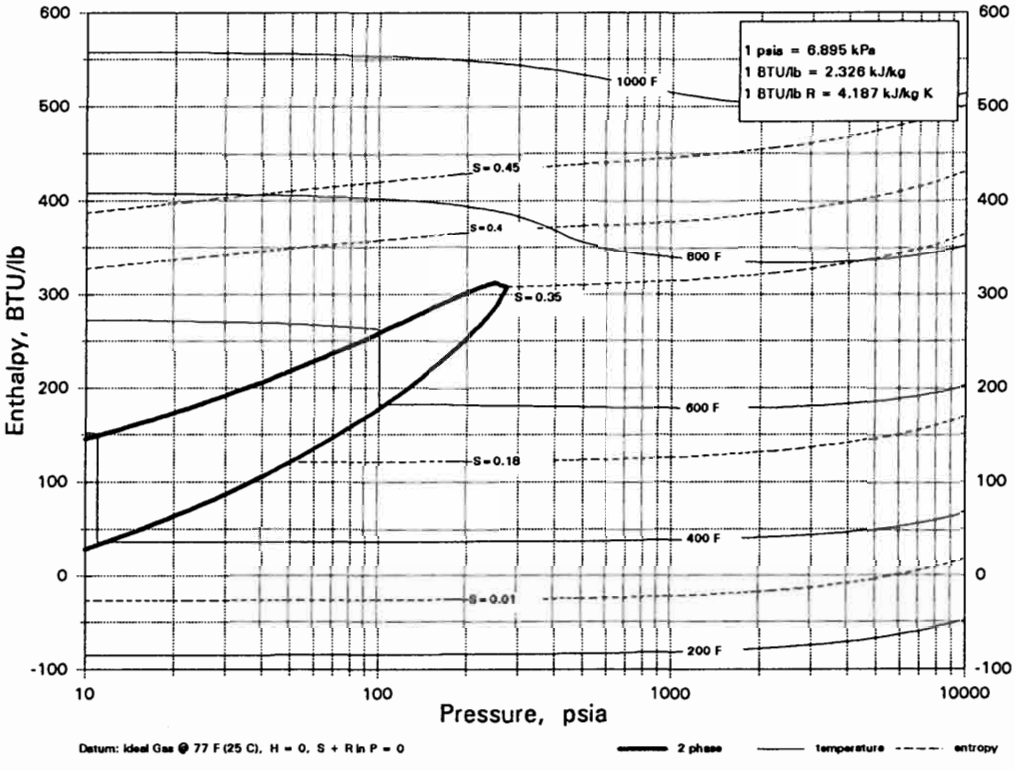
C12H23N DICYCLOHEXYLAMINE



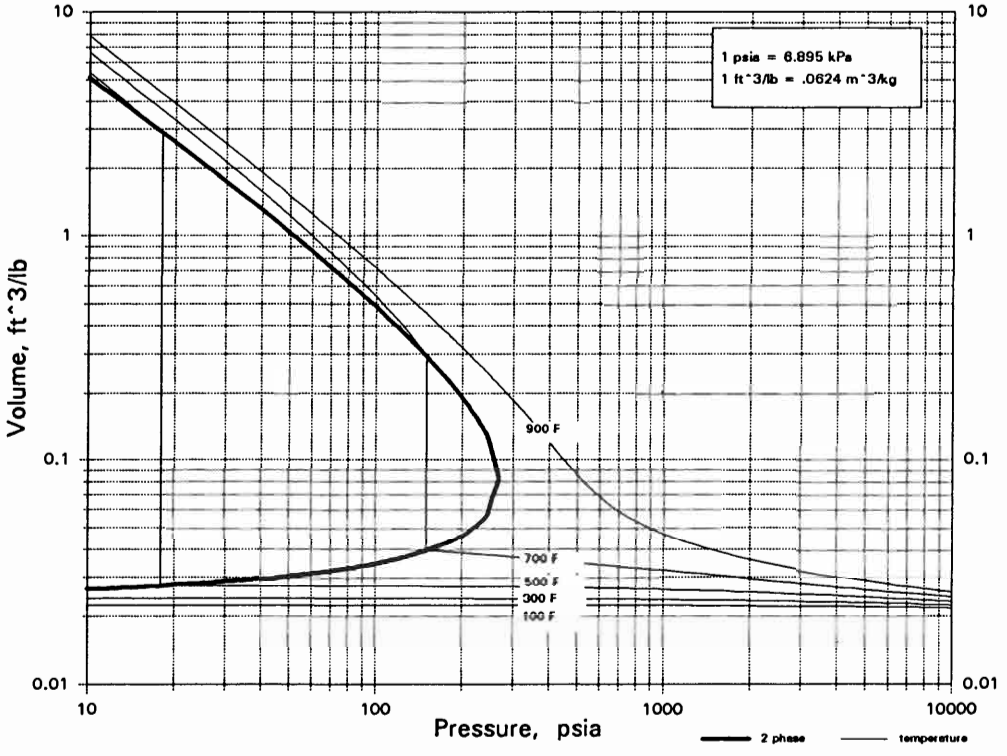


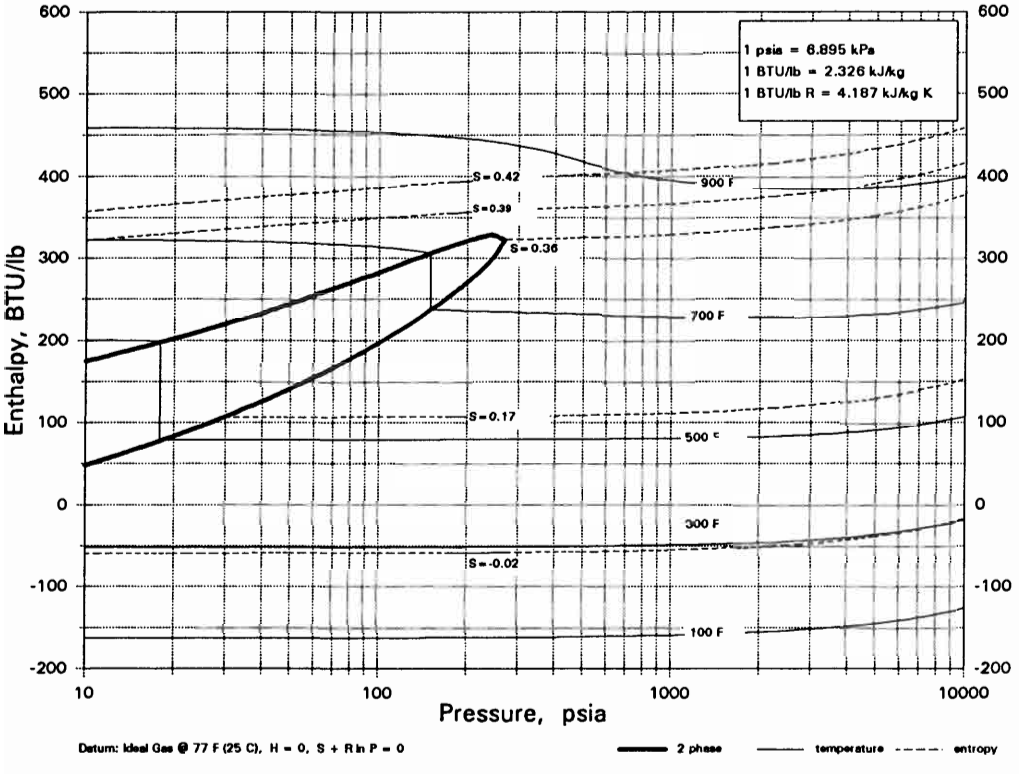
C12H24 1-DODECENE



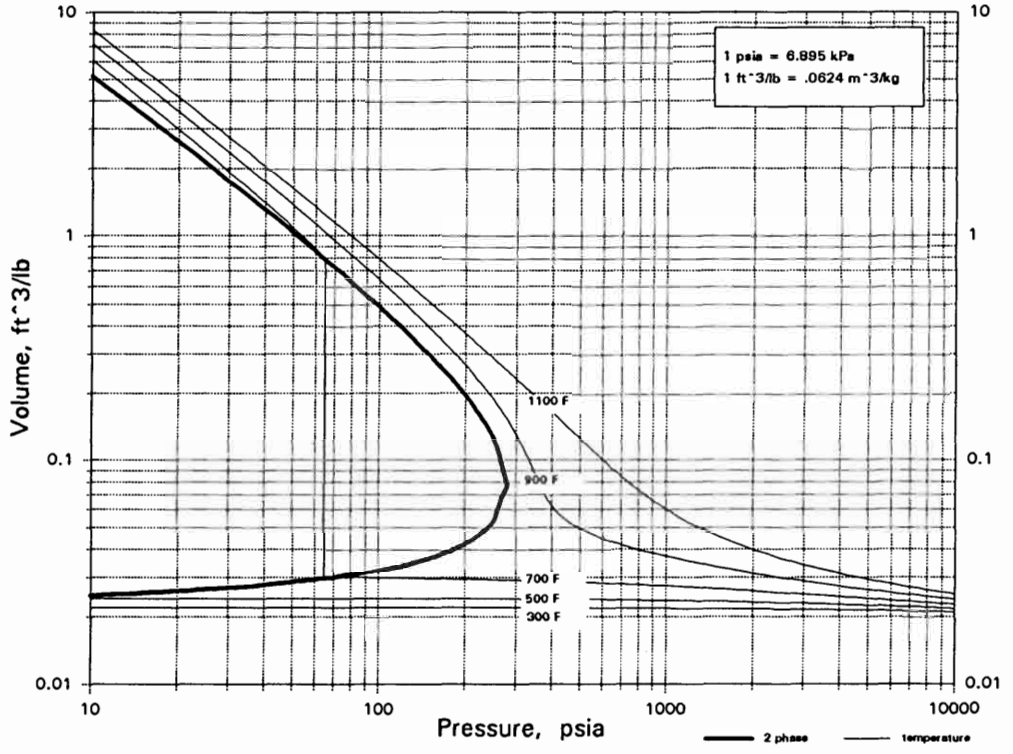


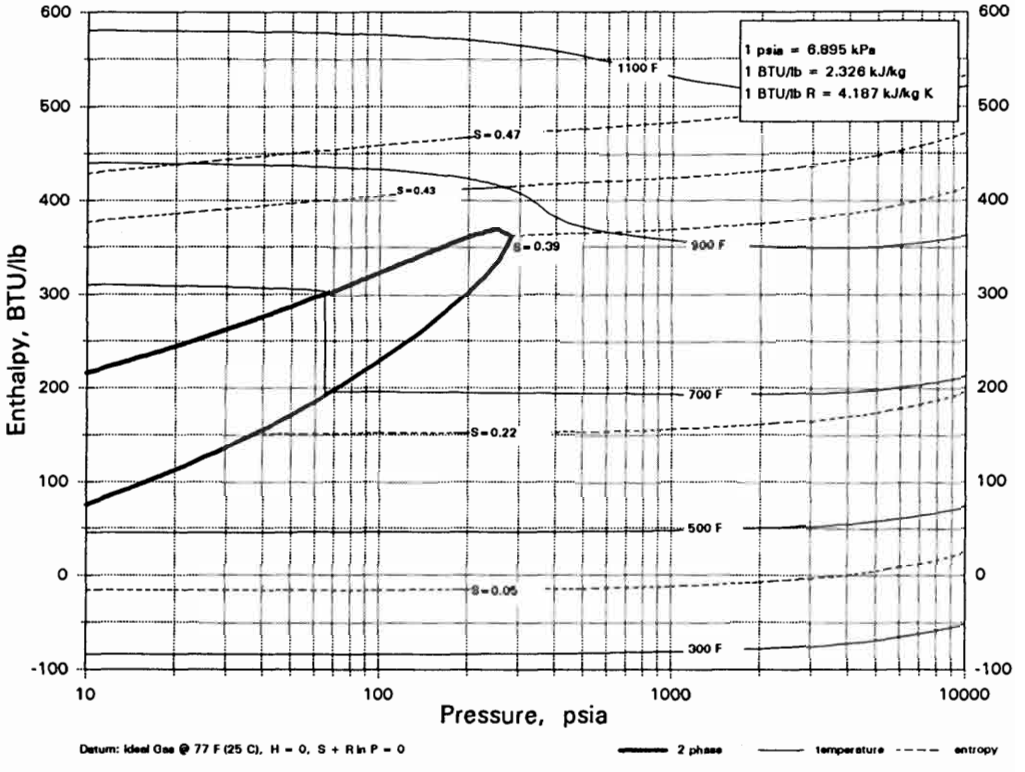
C12H24O 1-DODECANAL



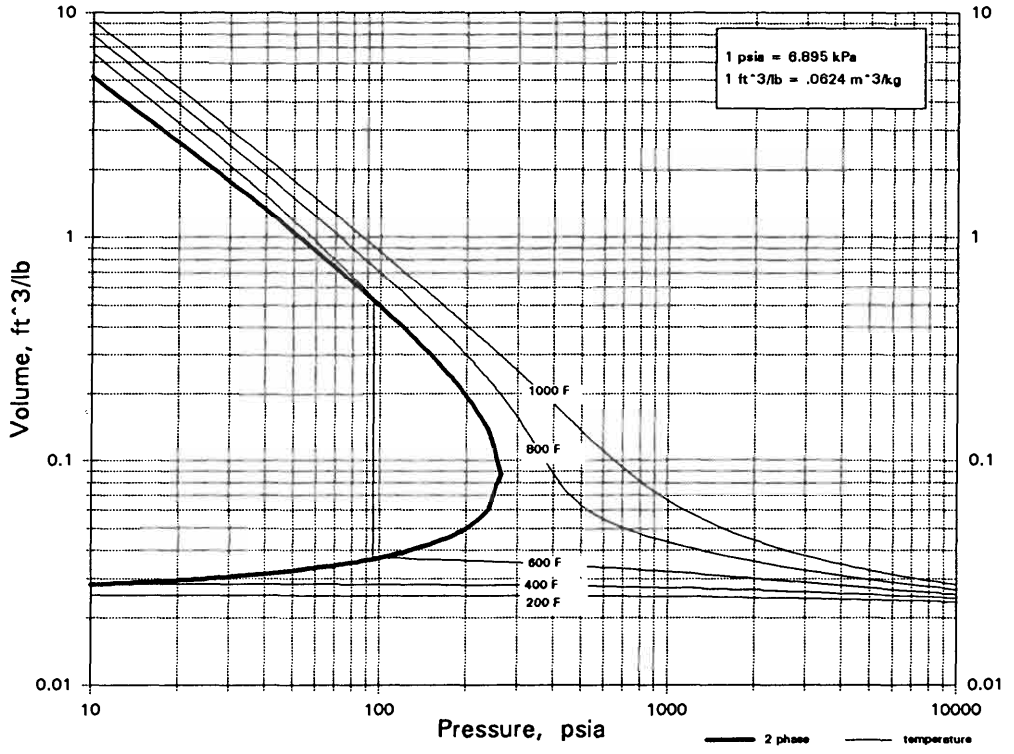


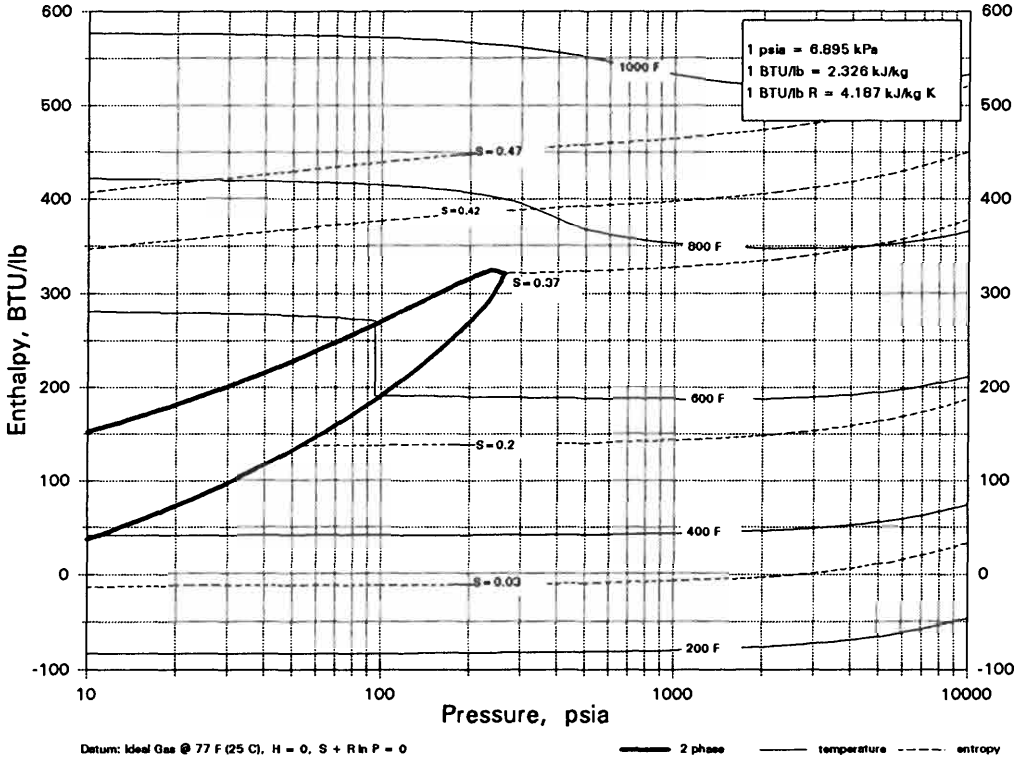
C12H24O2 n-DODECANOIC ACID



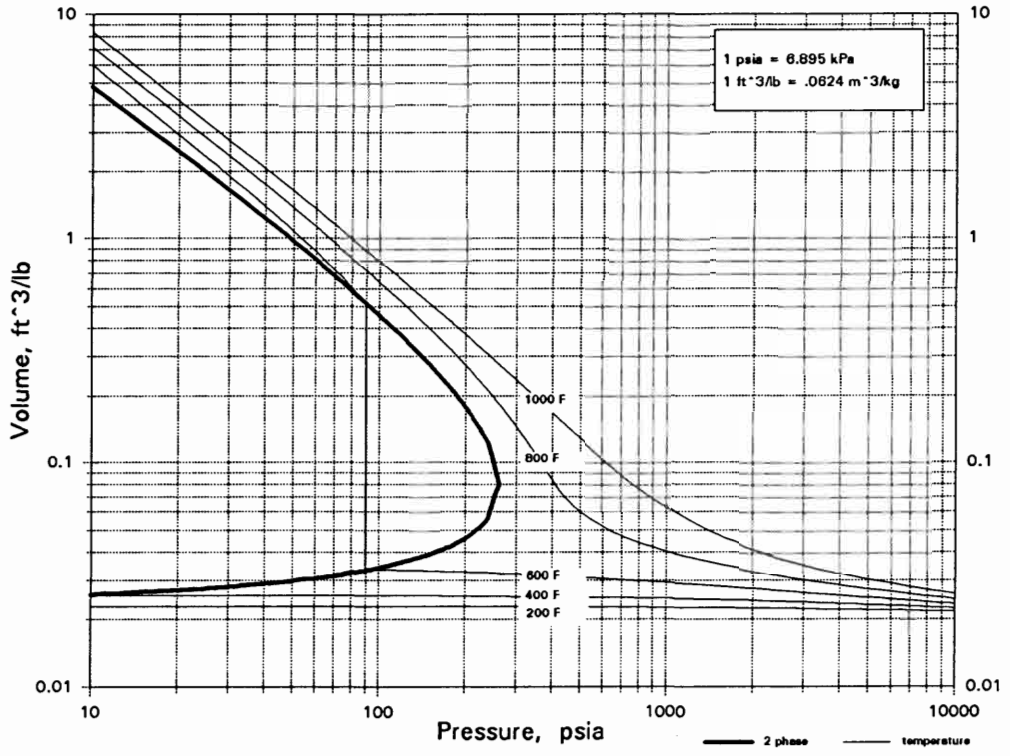


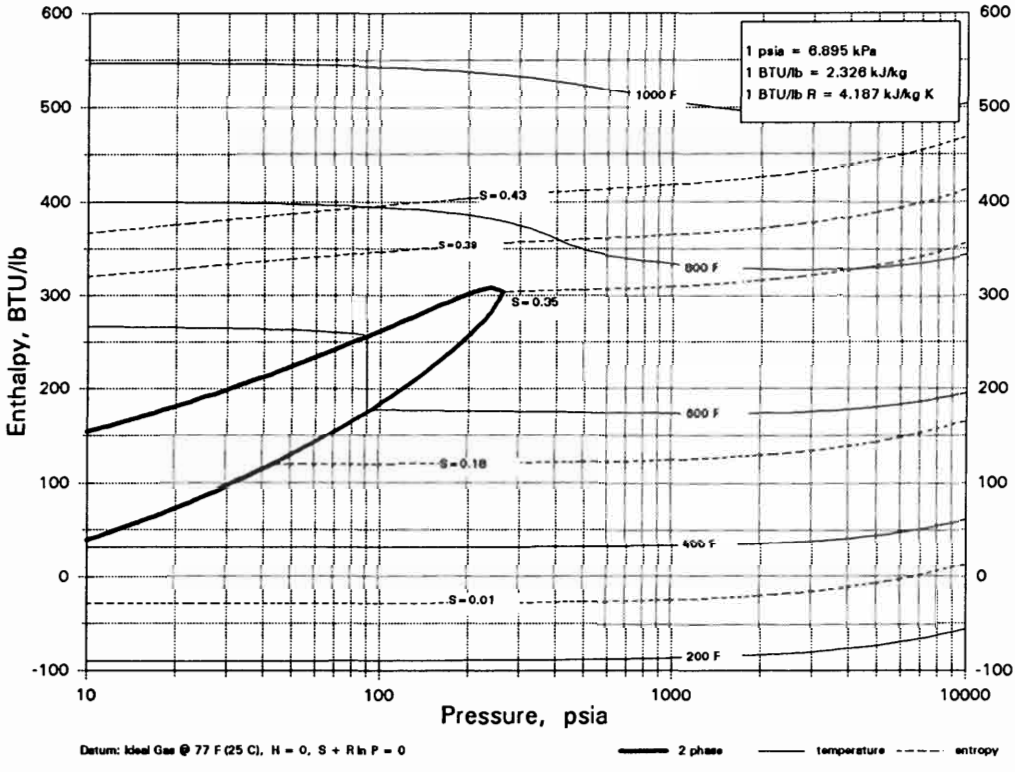
C12H26 n-DODECANE



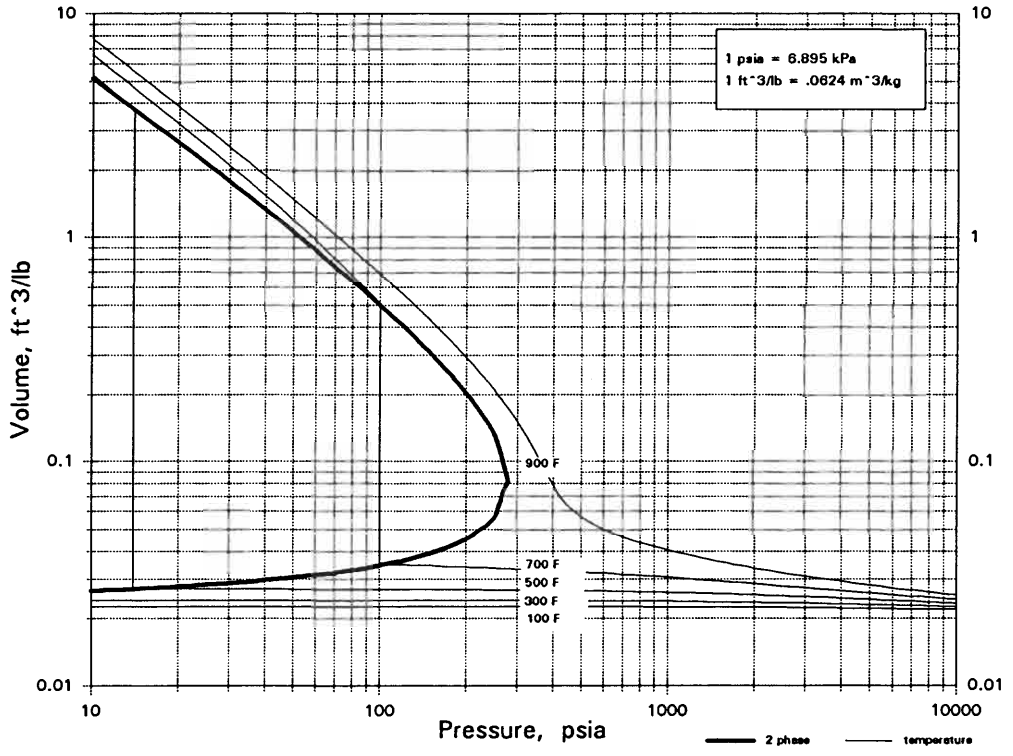


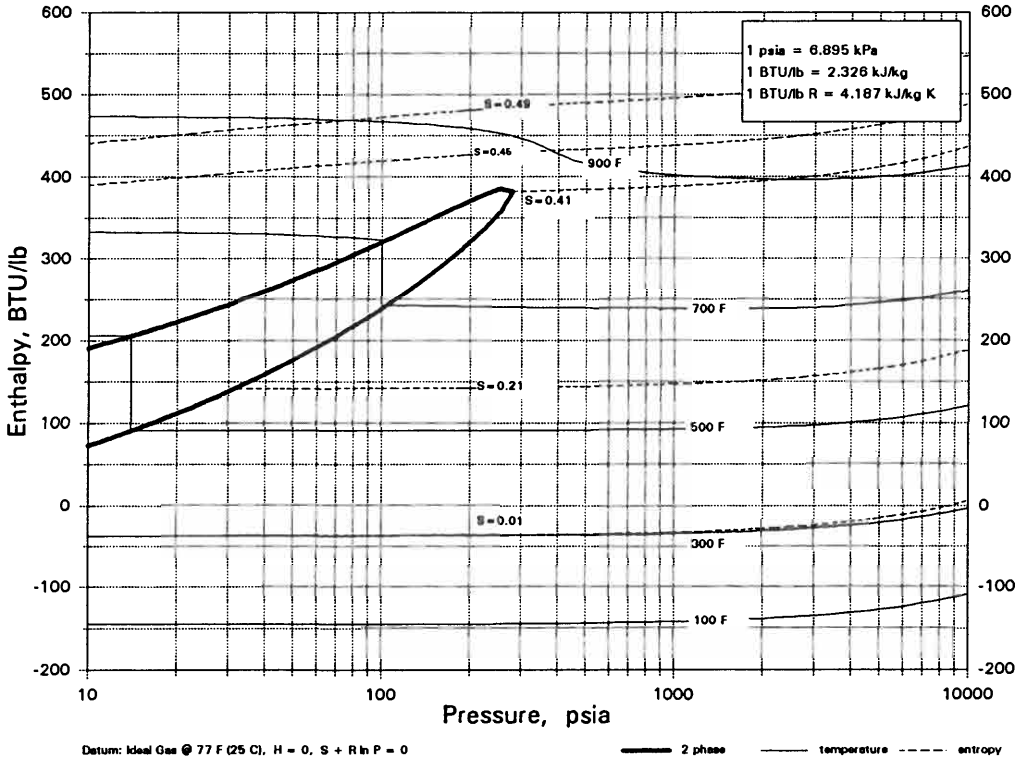
C12H26O DI-n-HEXYL ETHER



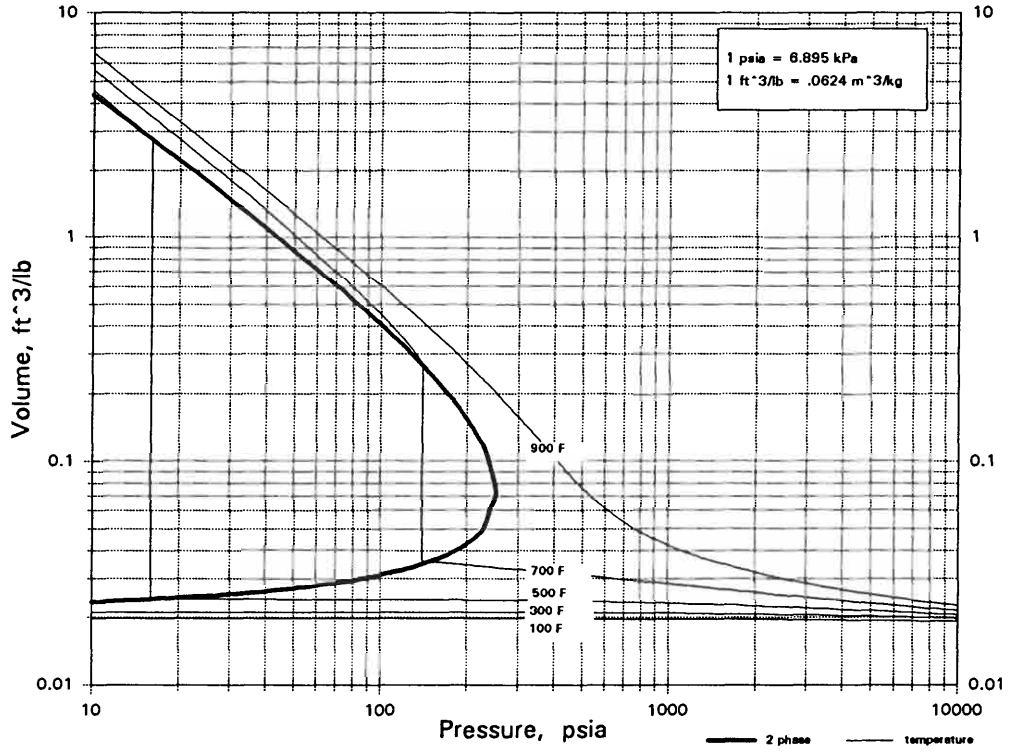


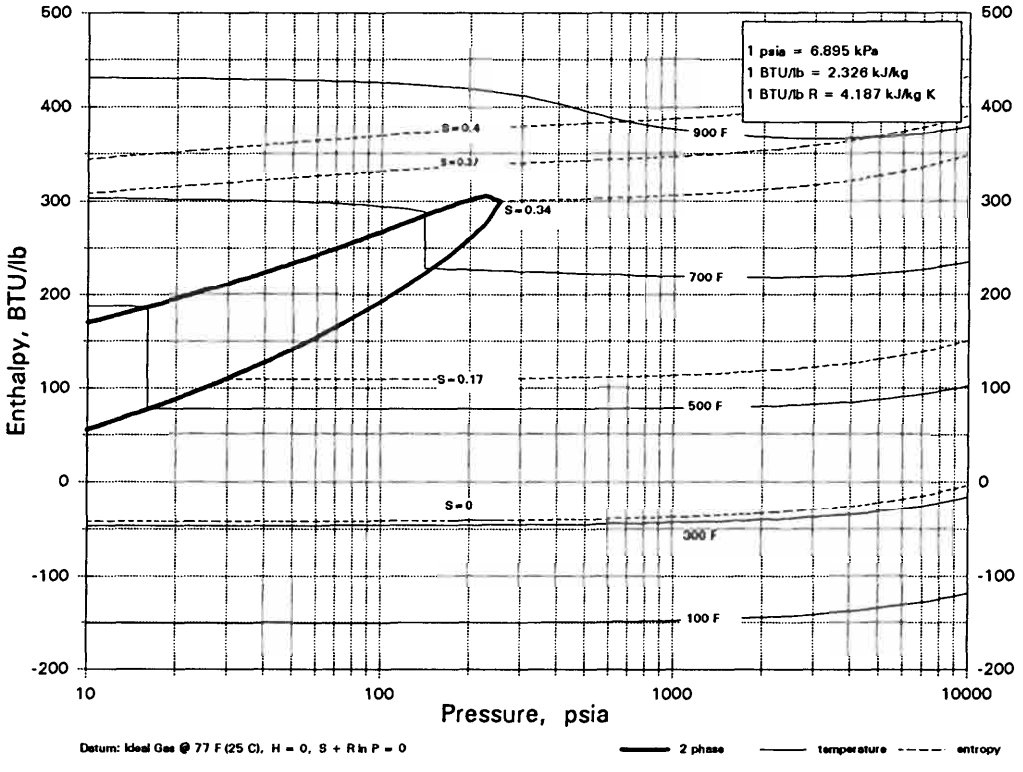
C12H26O 1-DODECANOL



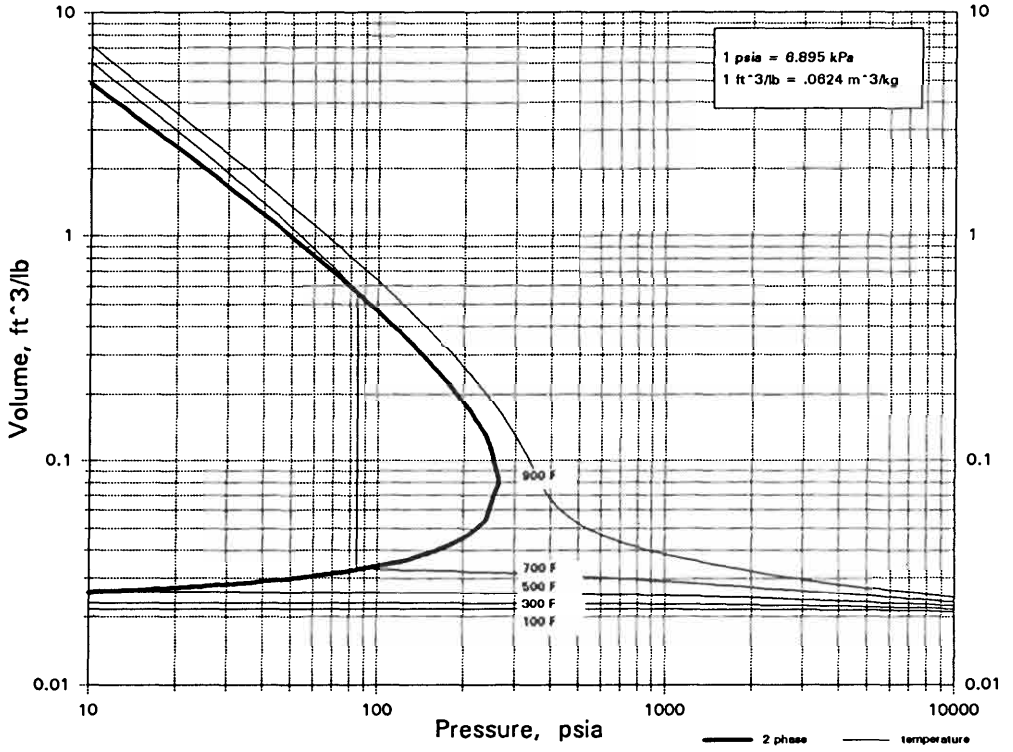


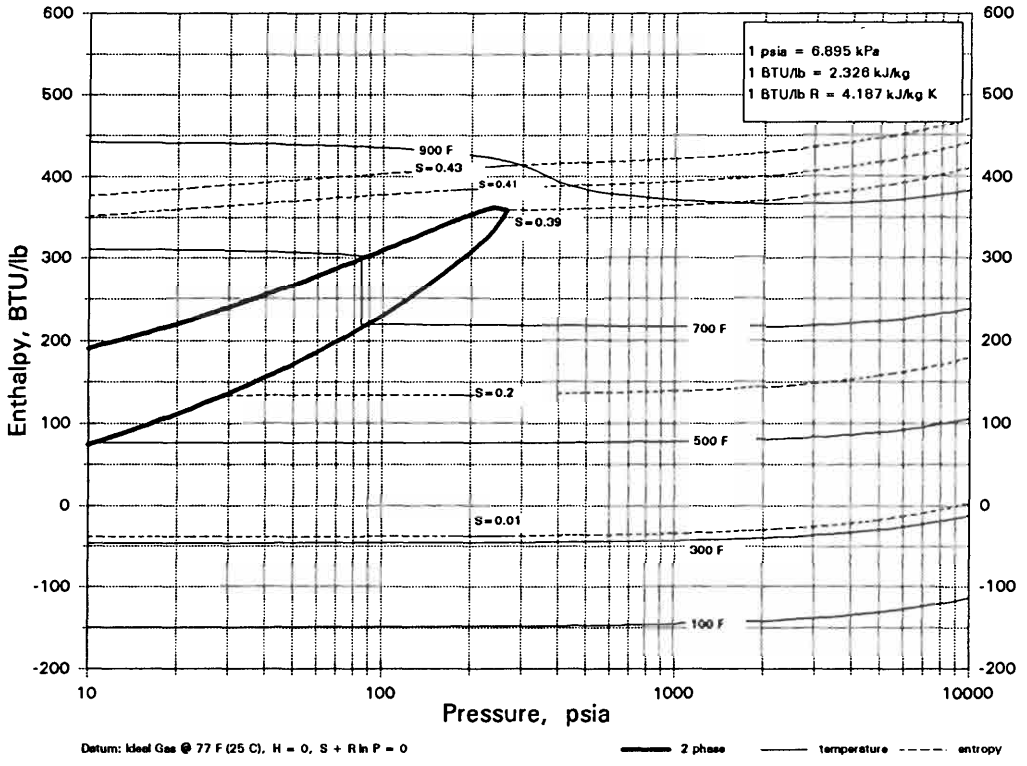
C12H26O3 DIETHYLENE GLYCOL DI-n-BUTYL ETHER



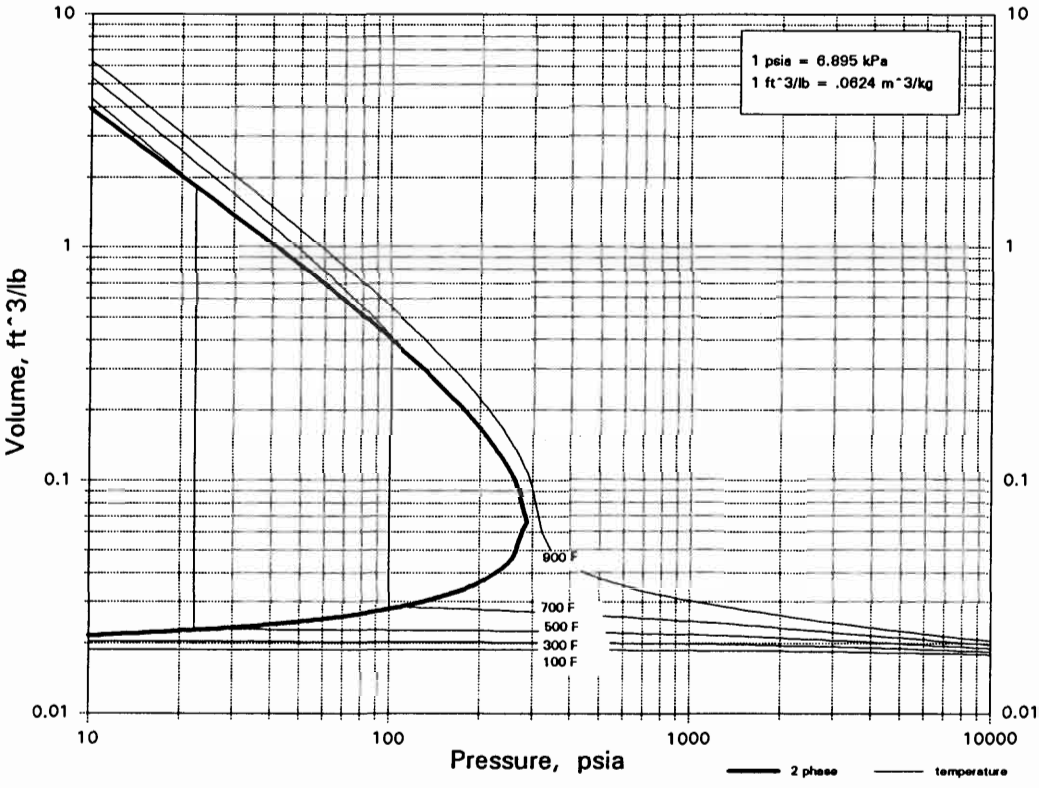


C12H26S n-DODECYL MERCAPTAN





C12H27BO3 TRI-n-BUTYL BORATE



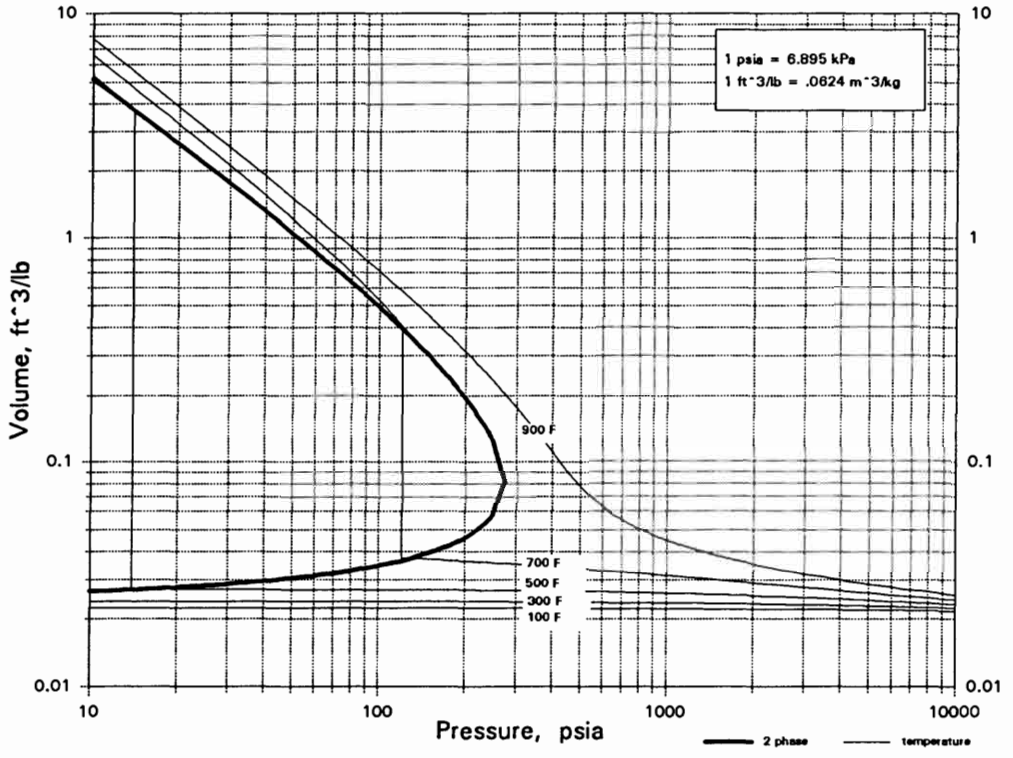
1. Boiling Point, K..... 506.65

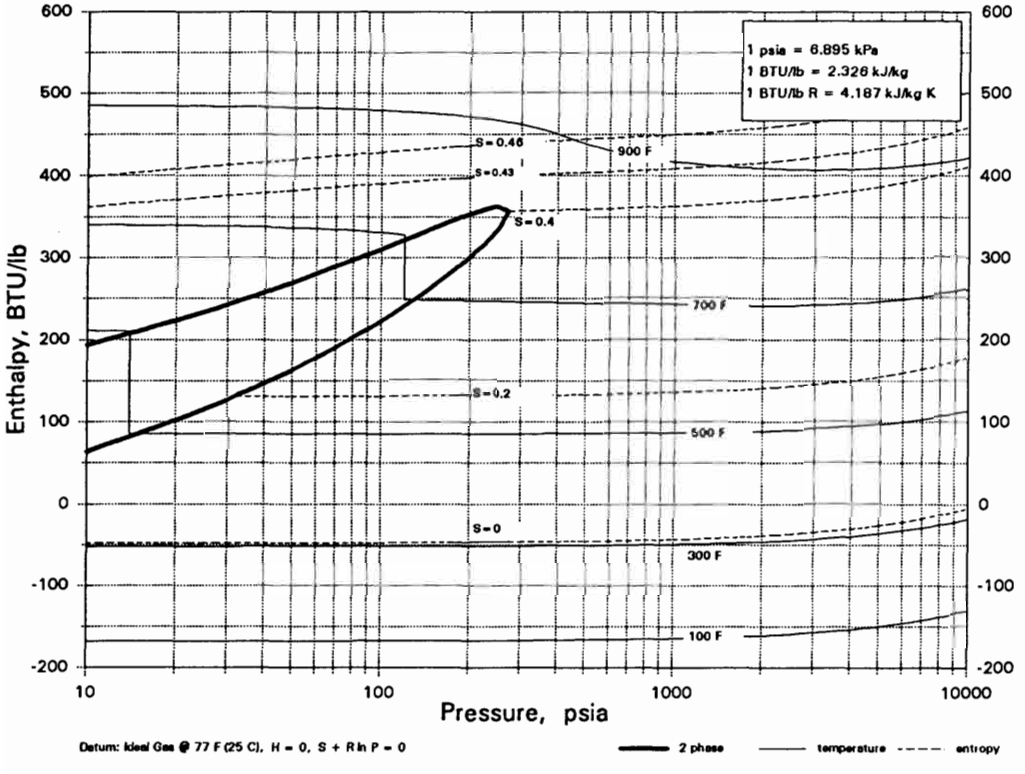
2. Critical Temperature, K.... 743.15

3. Critical Pressure, atm..... 19.63

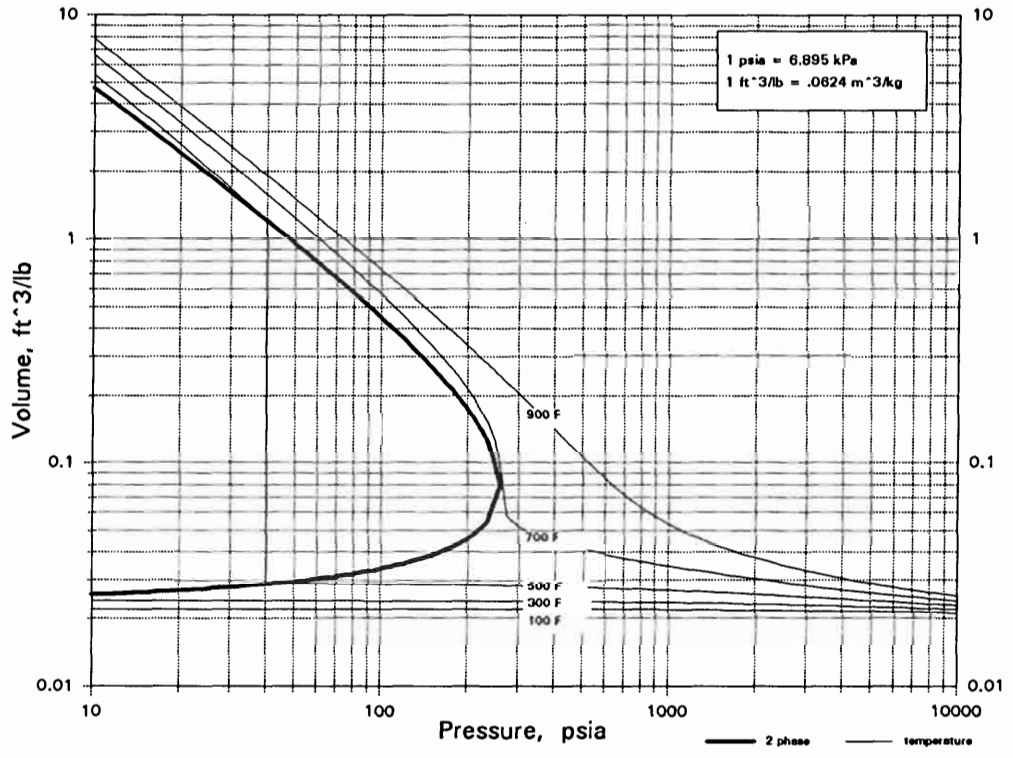
Heat capacity data are not available.

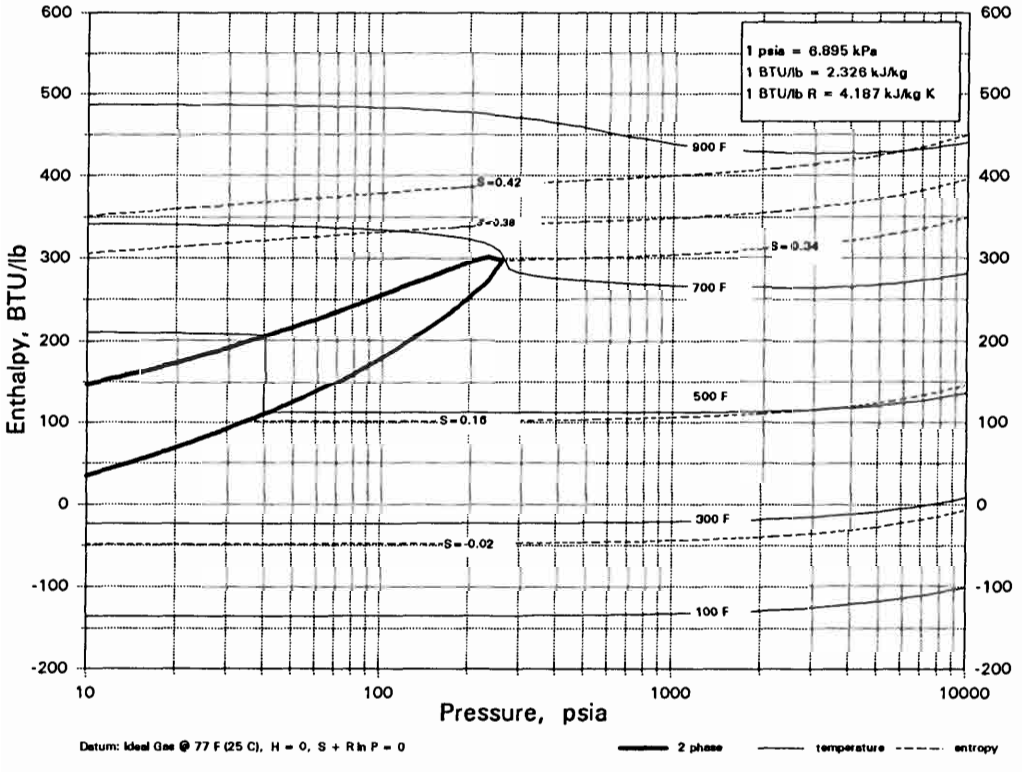
C12H27N DODECYLAMINE



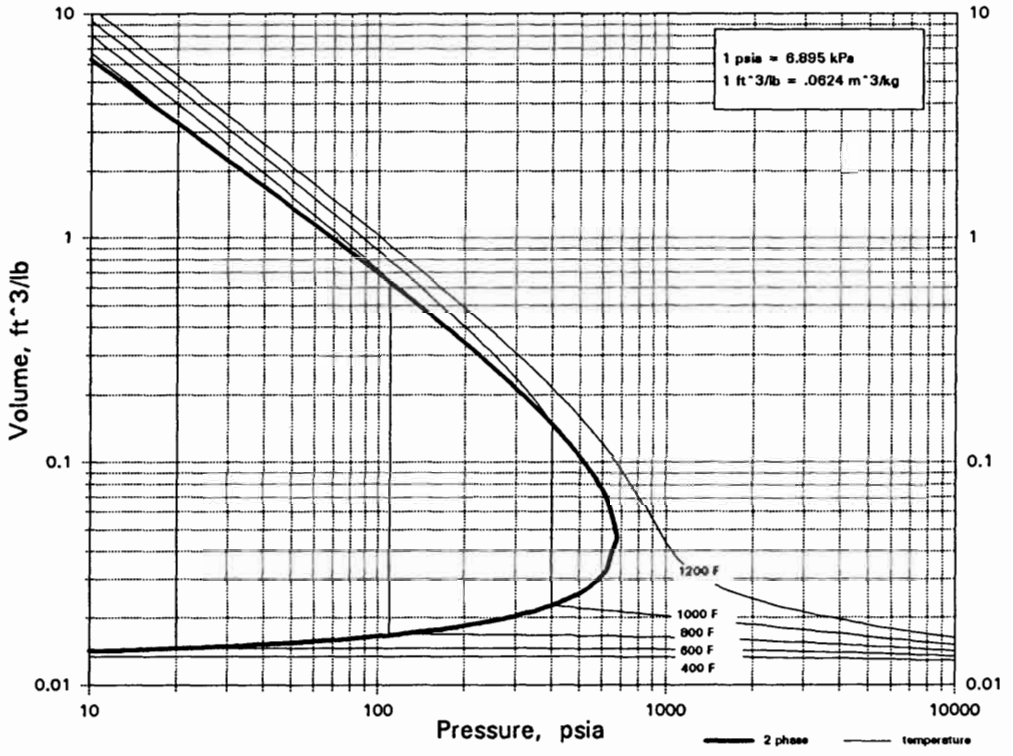


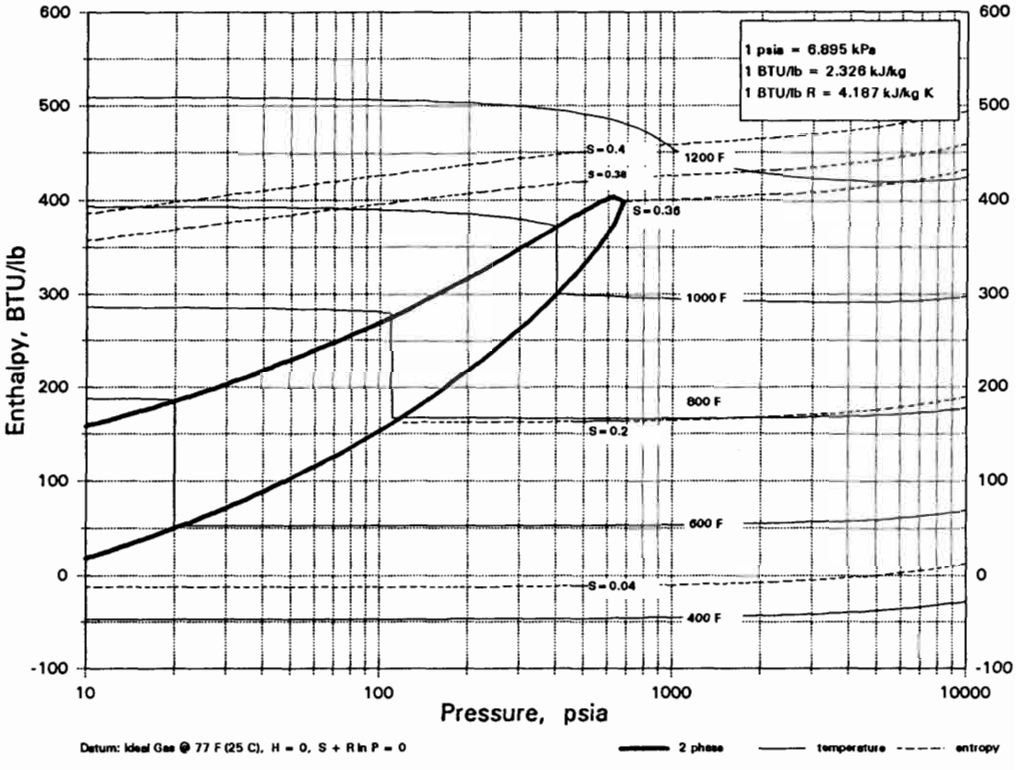
C12H27N TRI-n-BUTYLAMINE



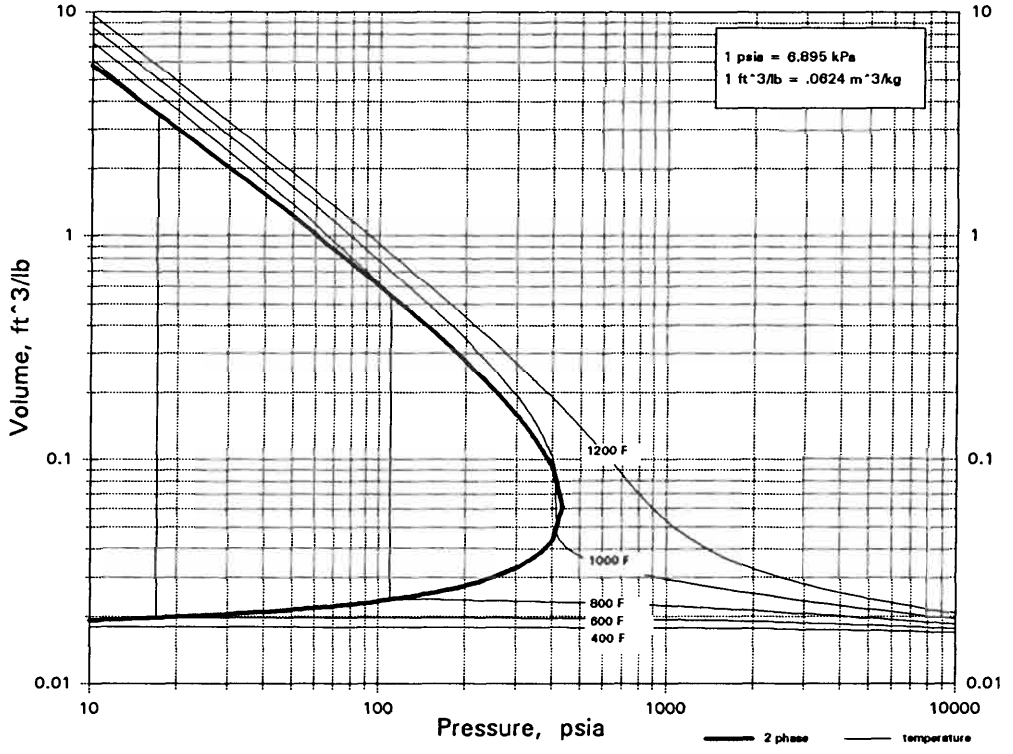


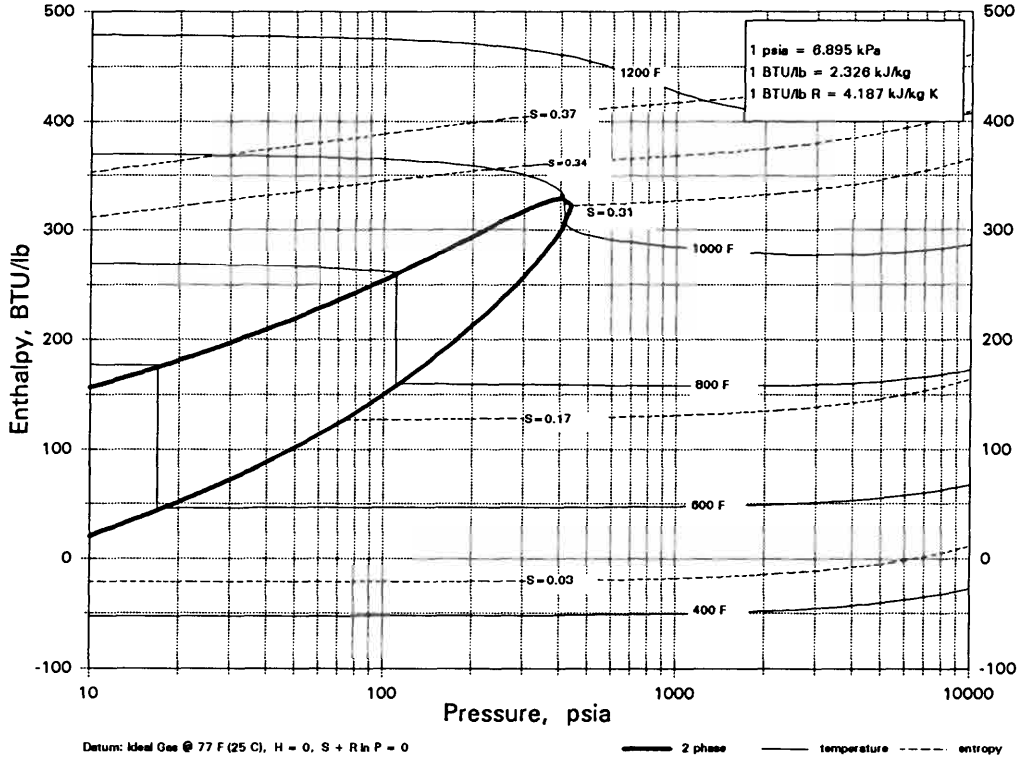
C13H10 FLUORENE



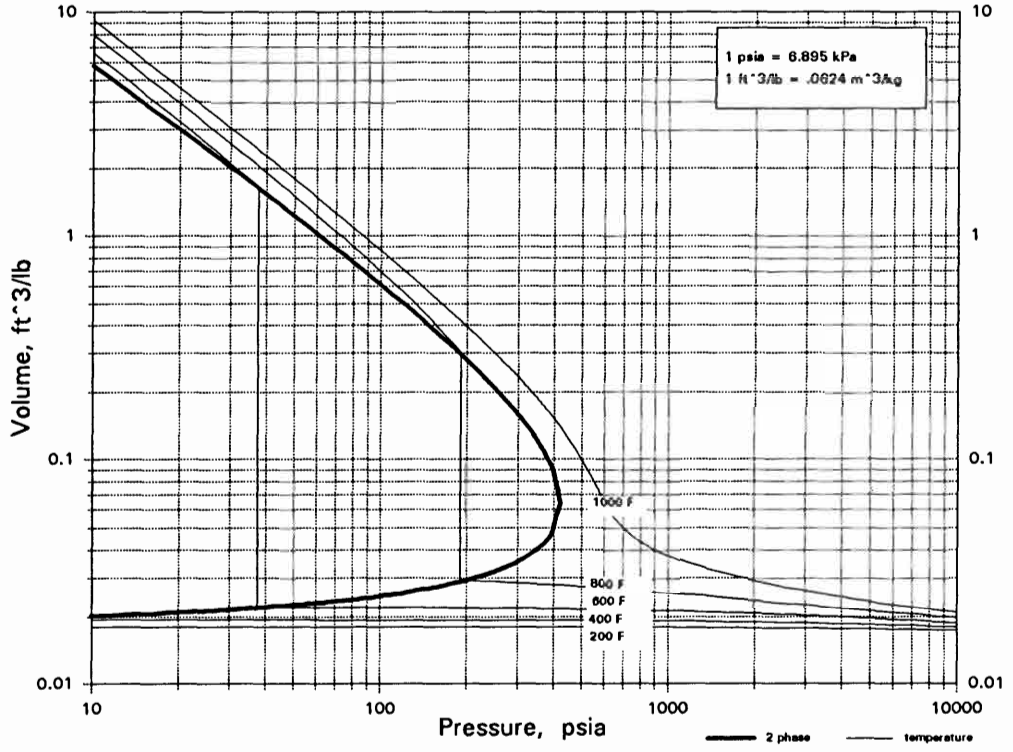


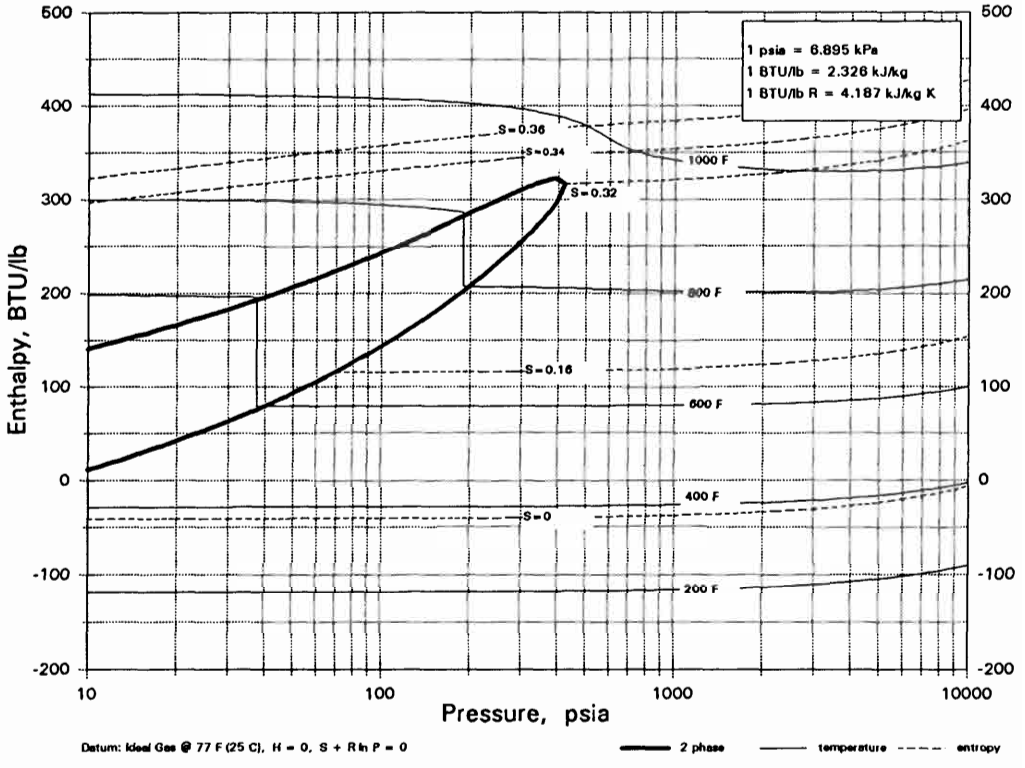
C13H10O BENZOPHENONE



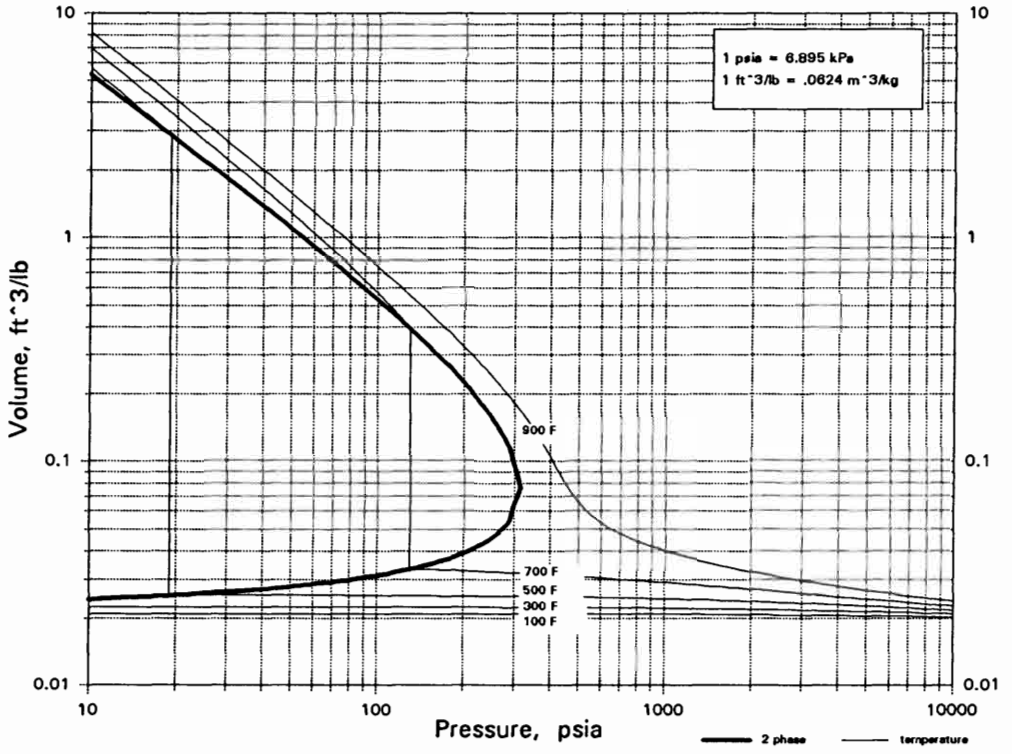


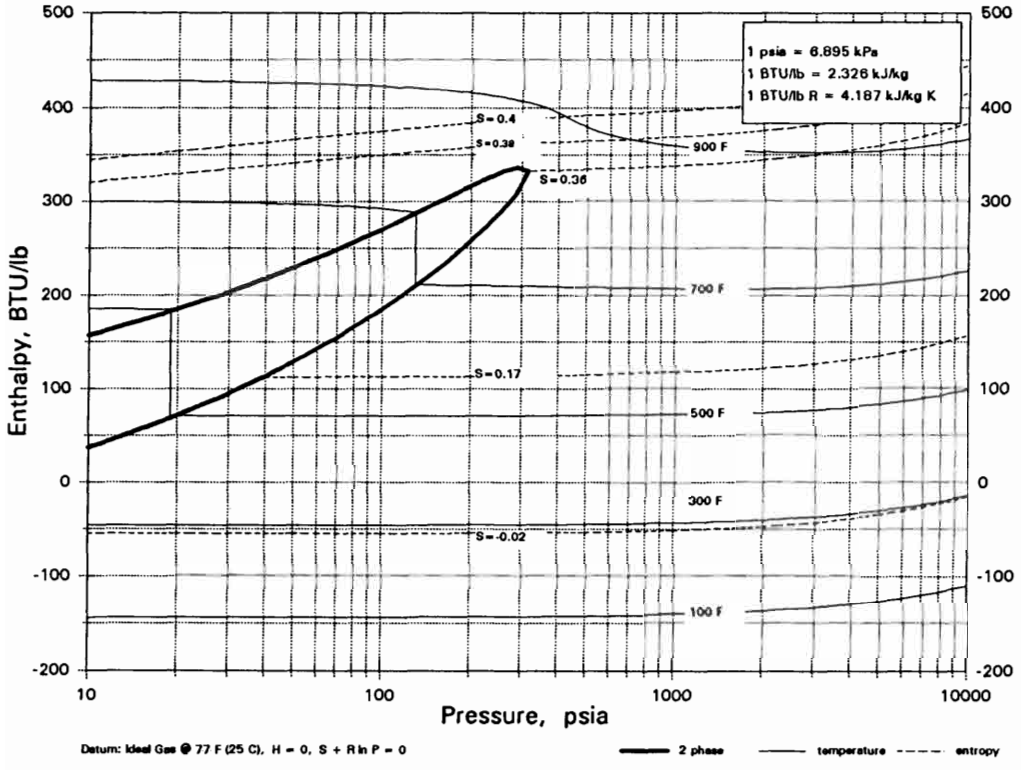
C13H12 DIPHENYLMETHANE



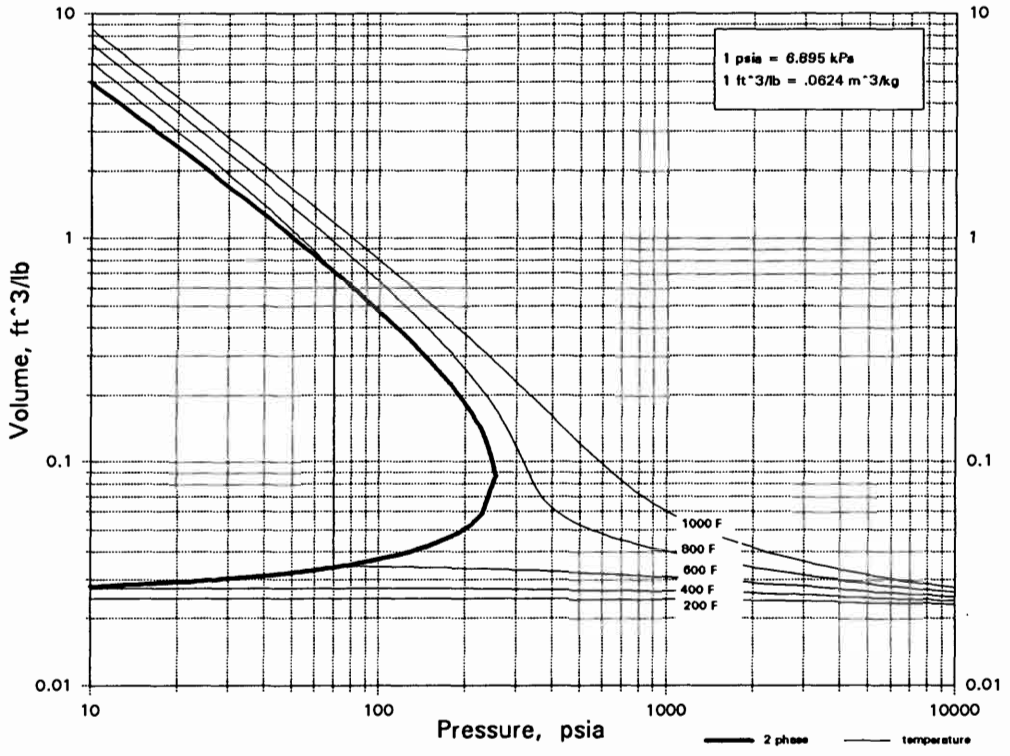


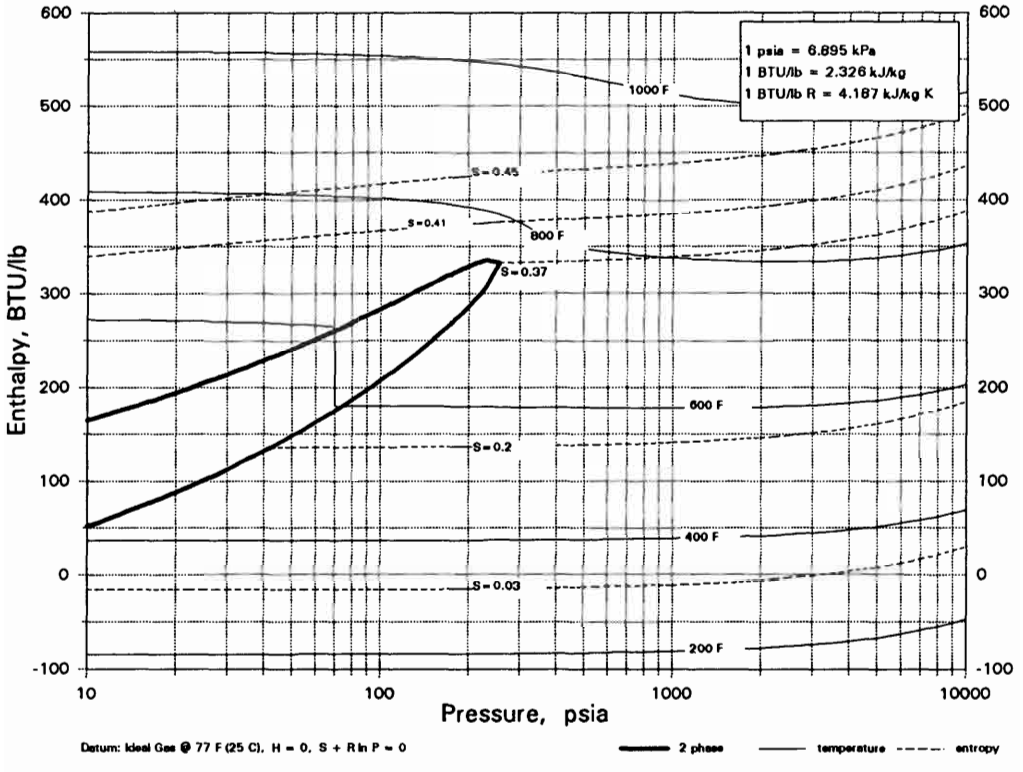
C13H20 n-HEPTYLBENZENE



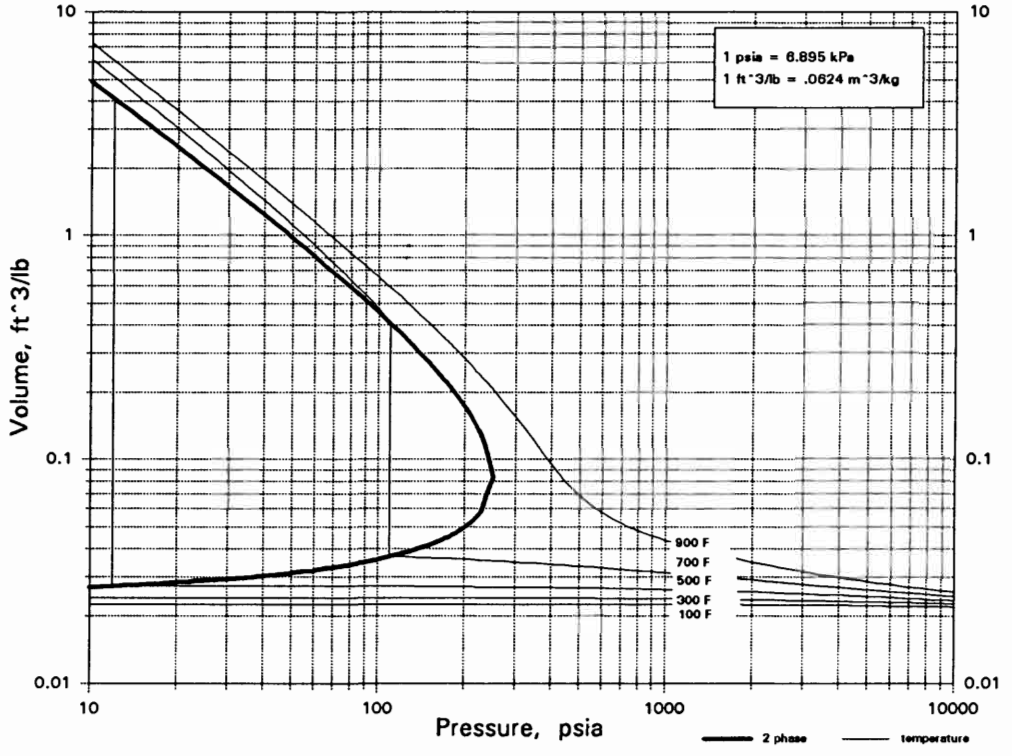


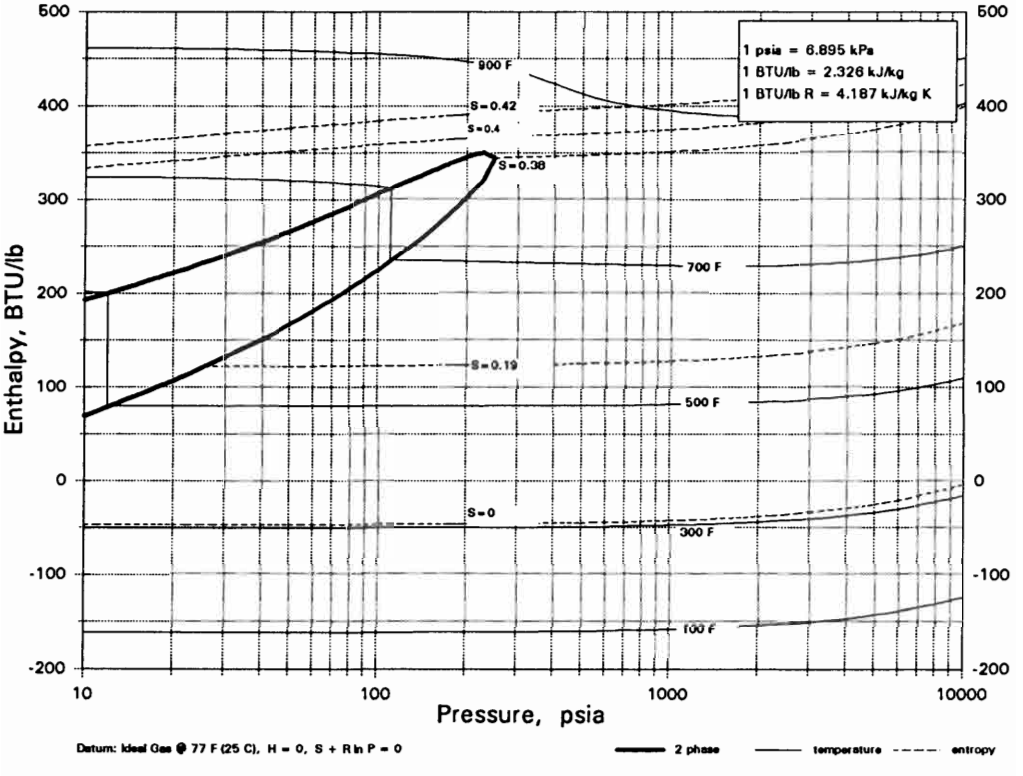
C13H26 1-TRIDECENE



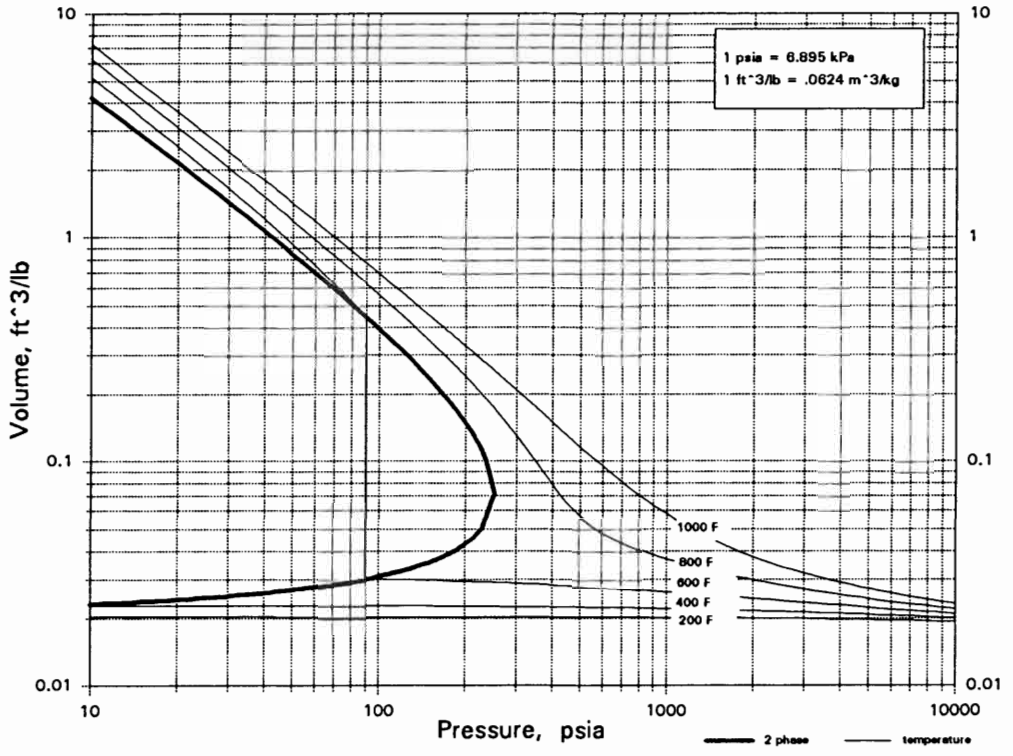


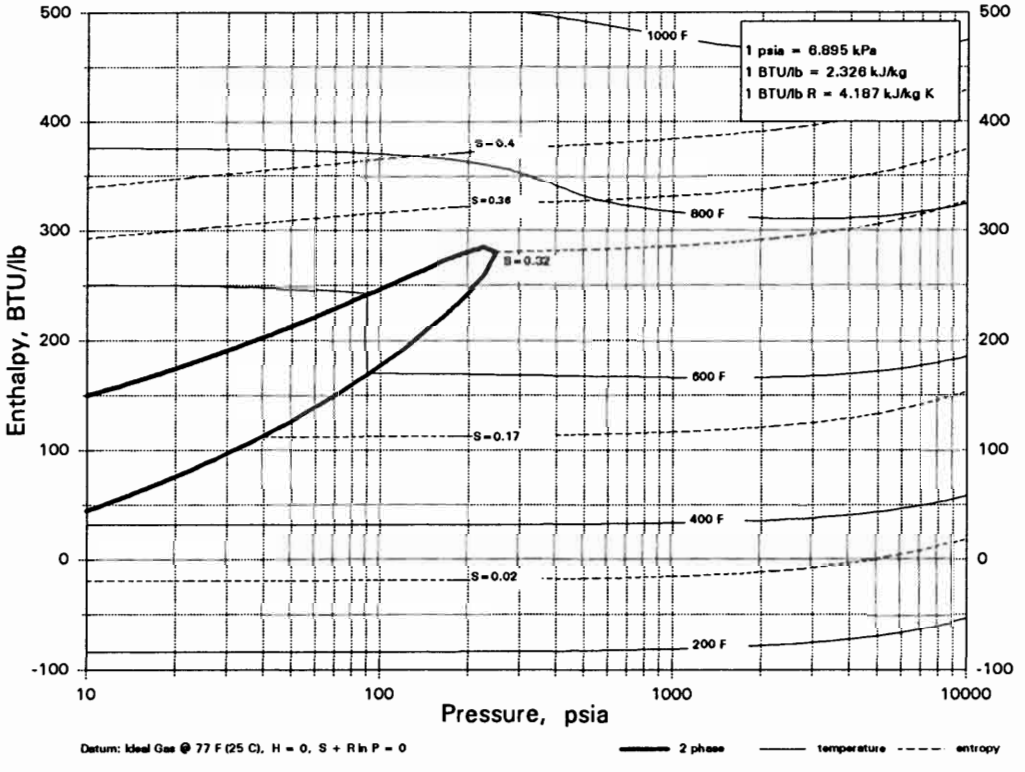
C13H26O 1-TRIDECANAL



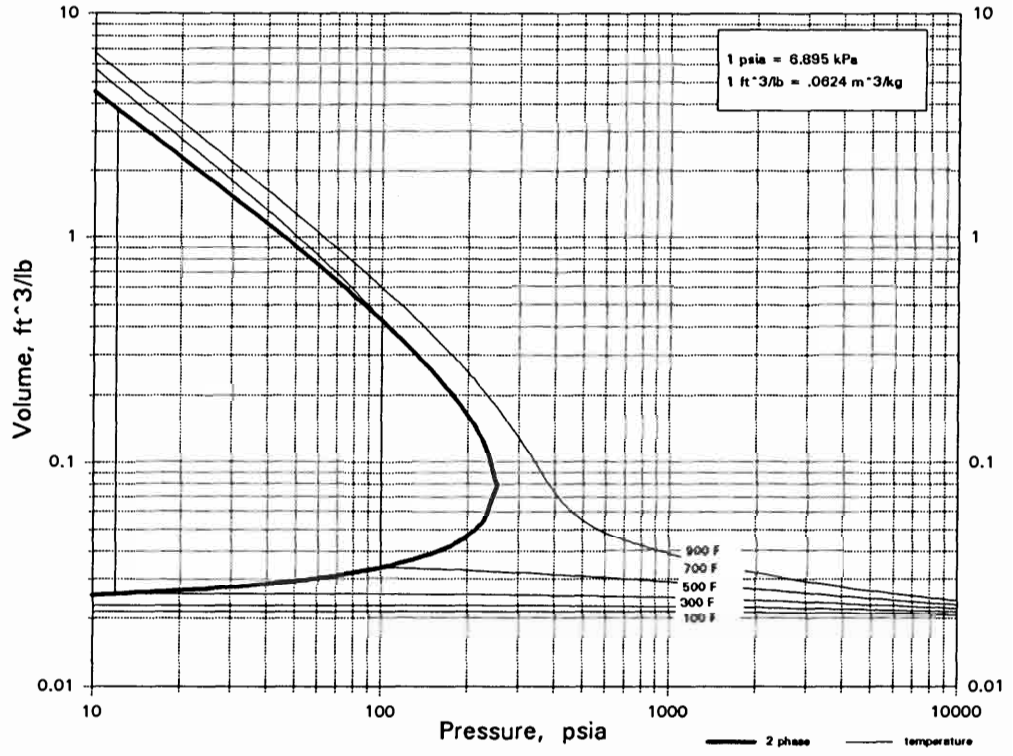


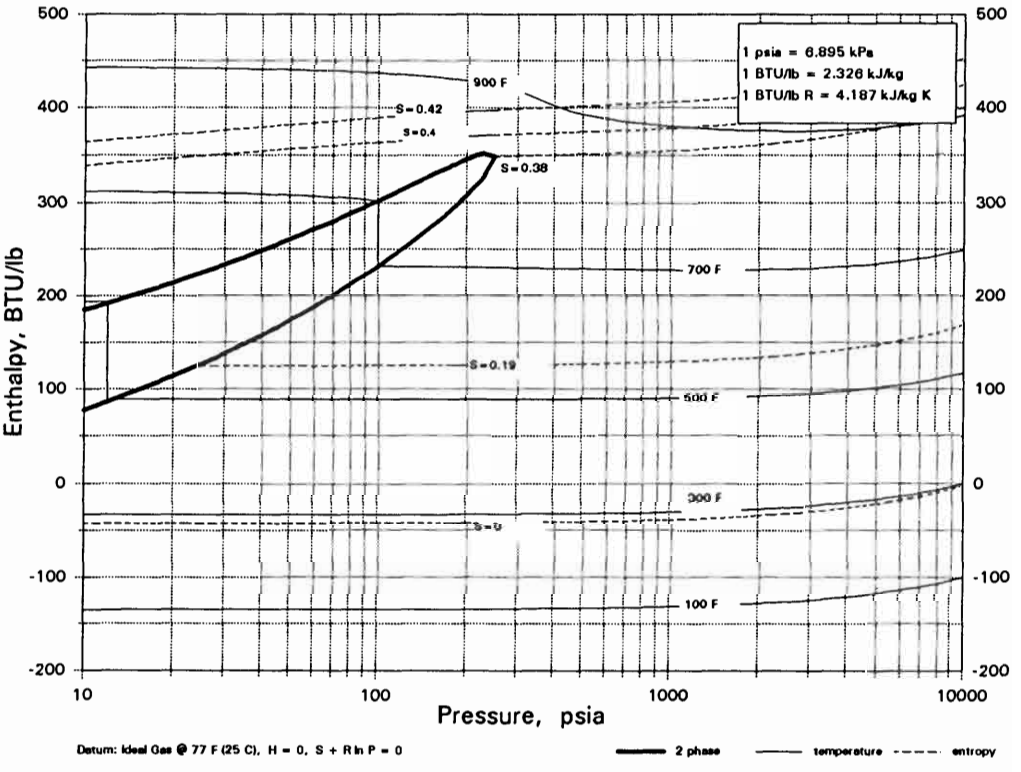
C13H26O2 n-BUTYL NONANOATE



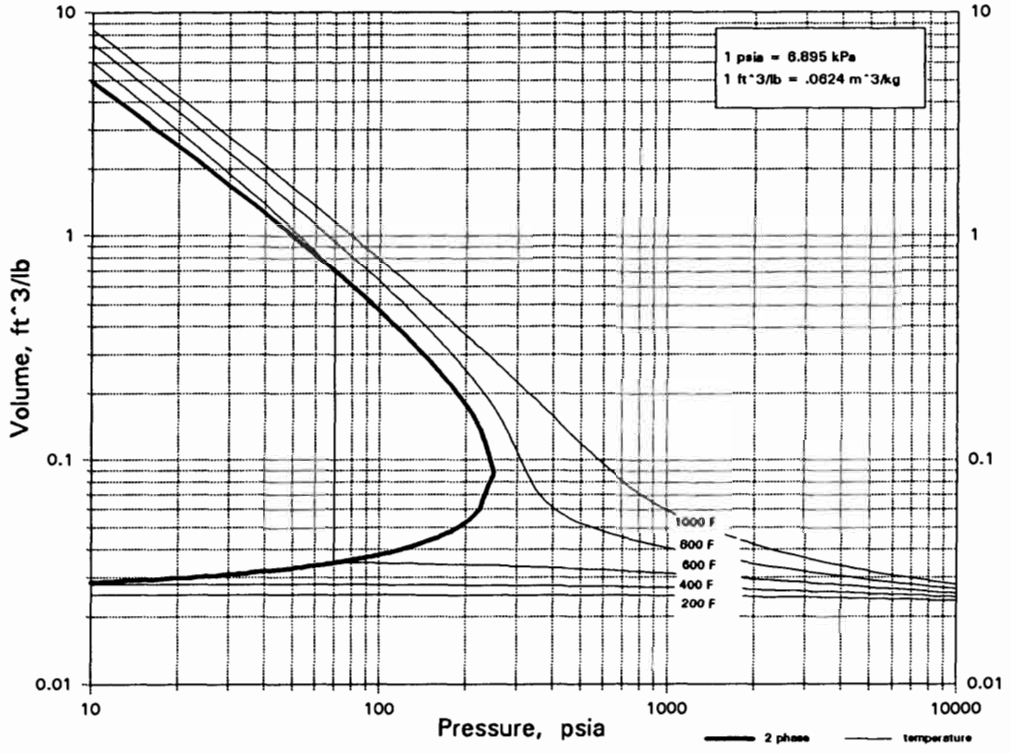


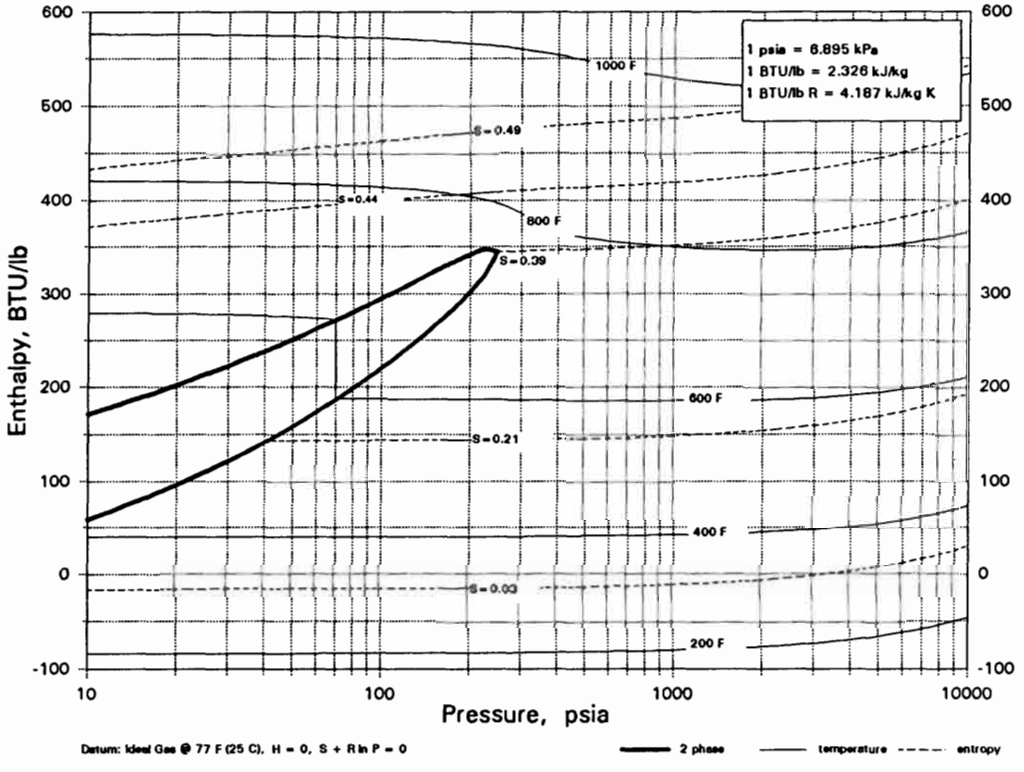
C13H26O2 METHYL DODECANOATE



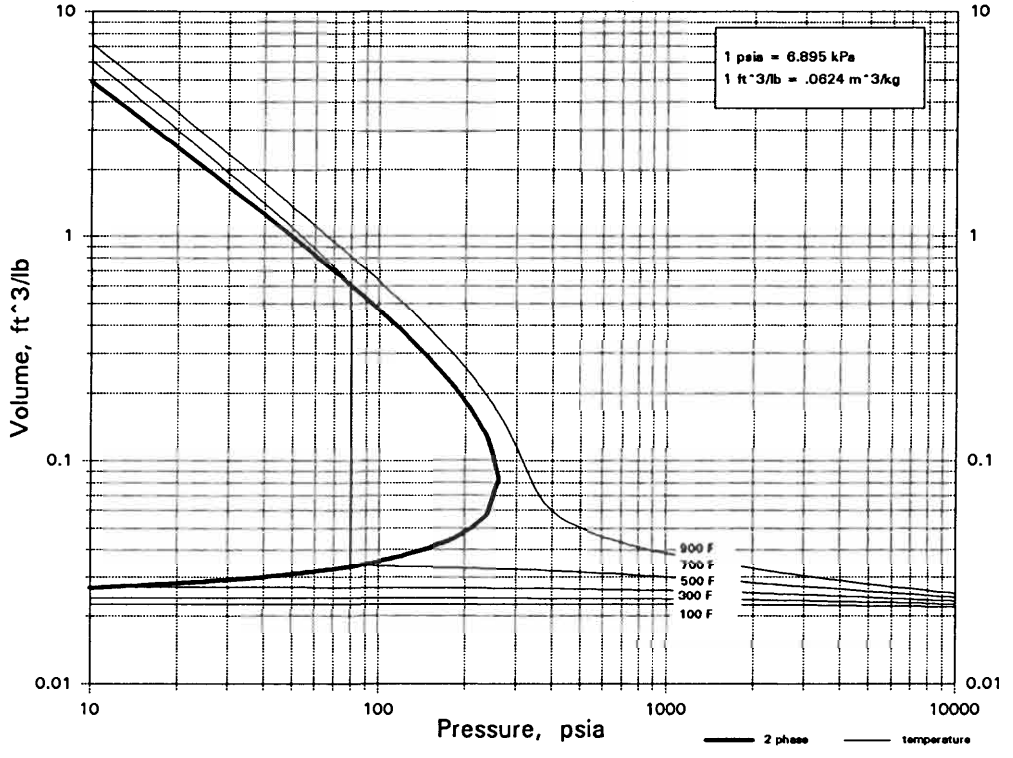


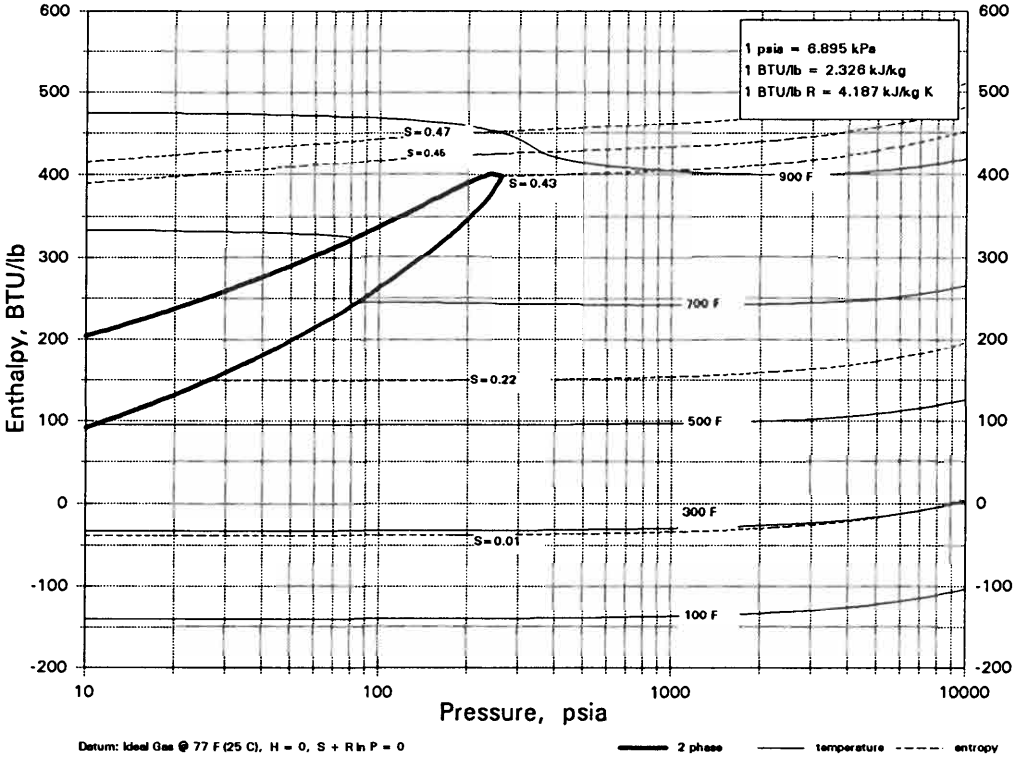
C13H28 n-TRIDECANE



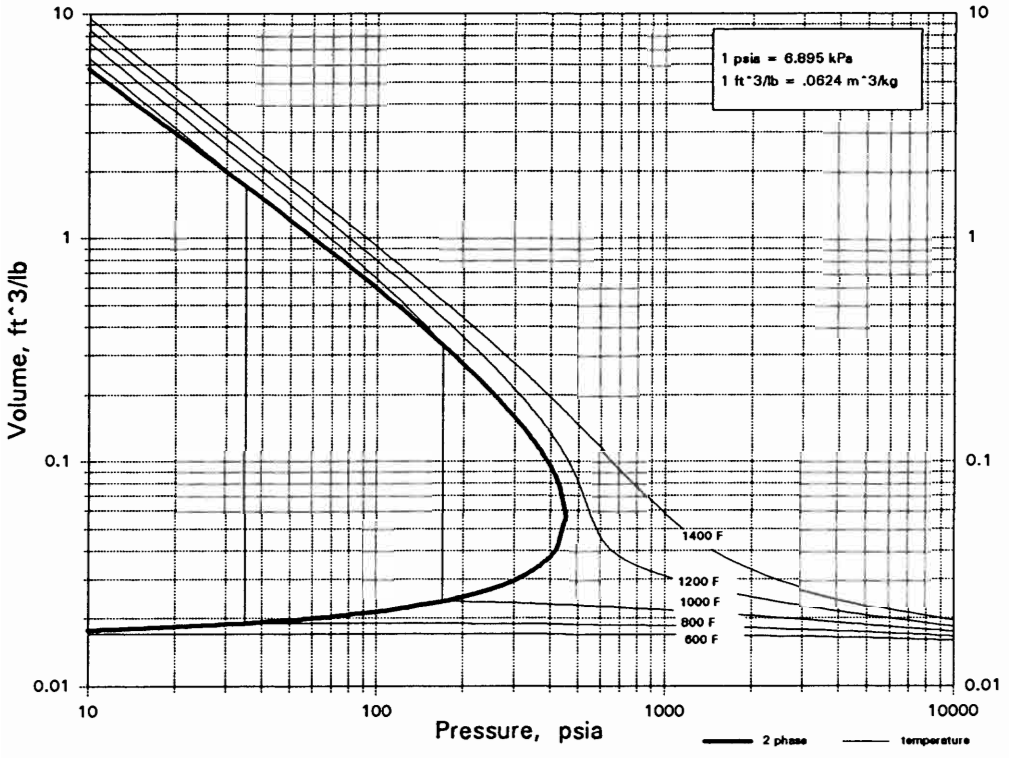


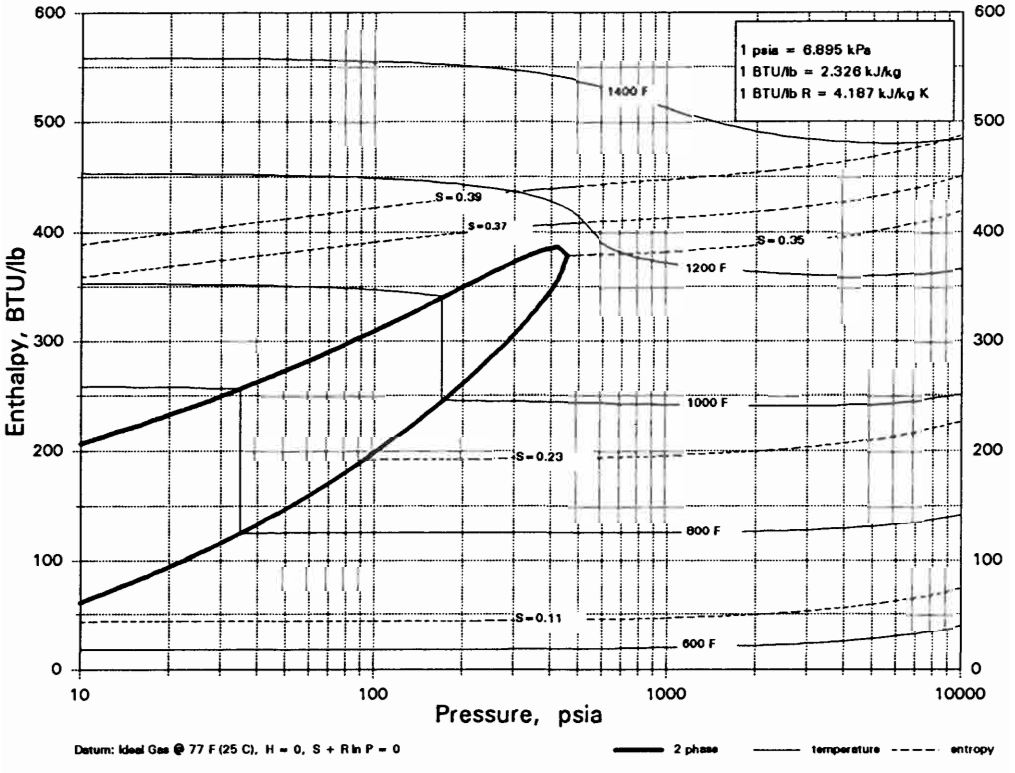
C13H28O 1-TRIDECANOL



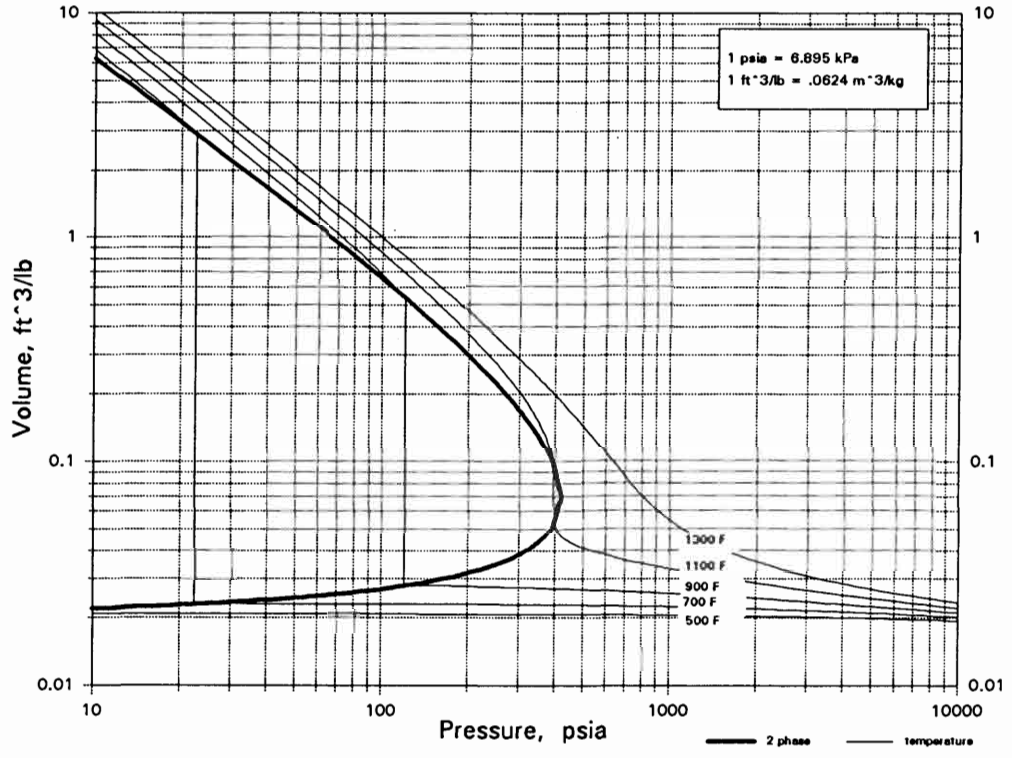


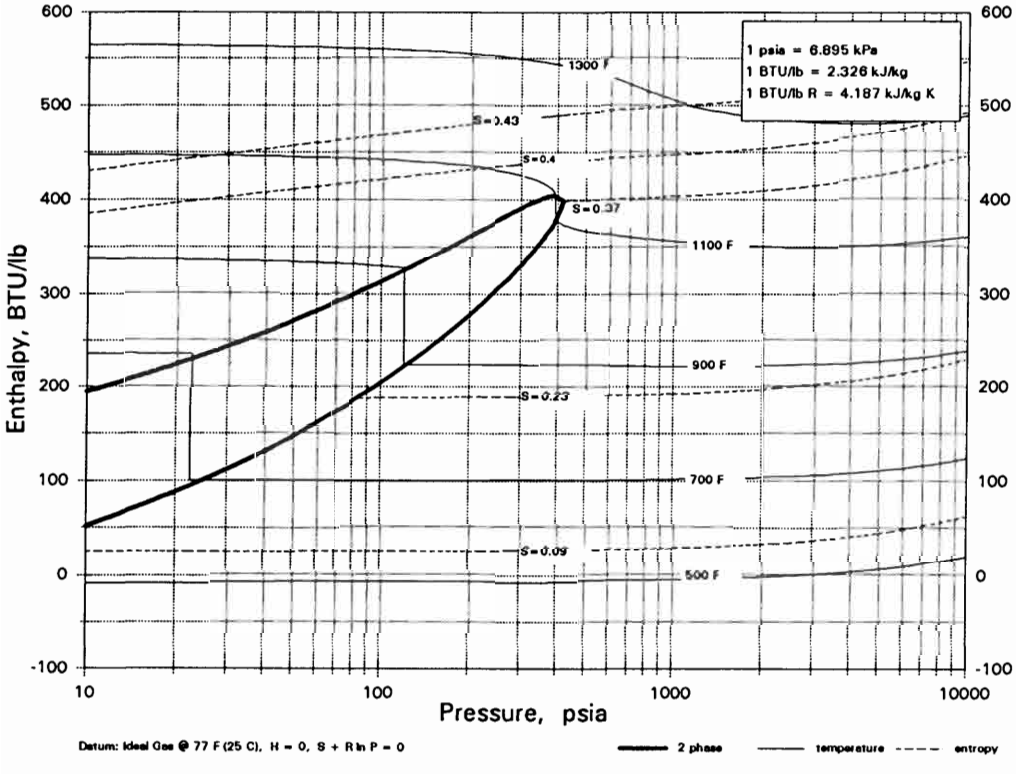
C14H8O2 ANTHRAQUINONE



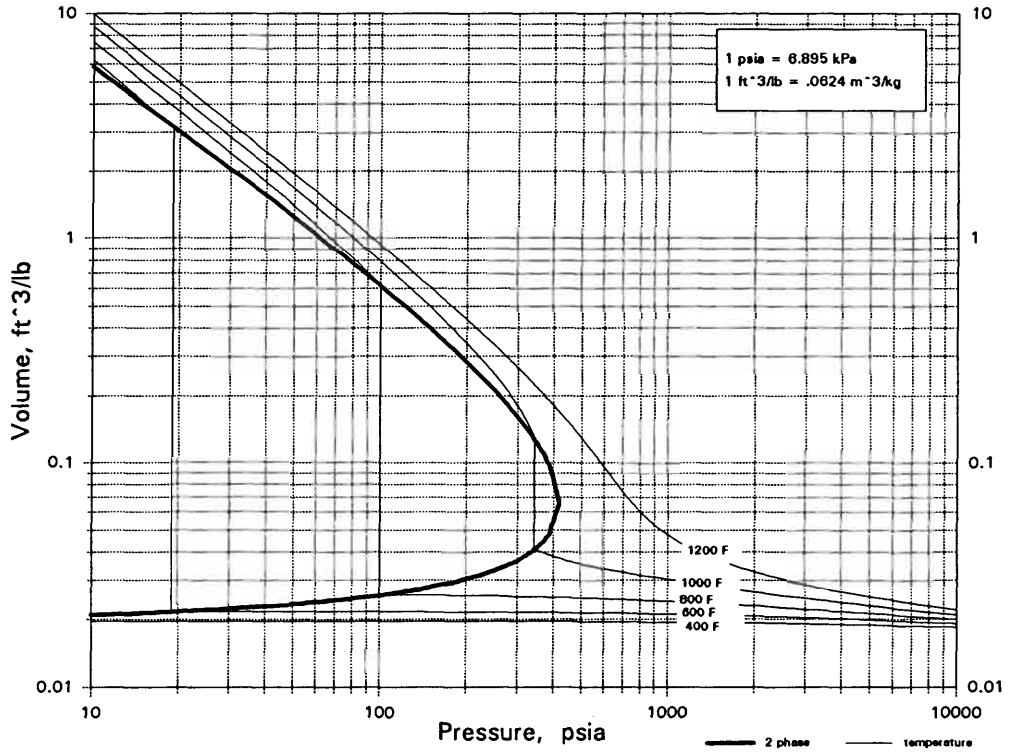


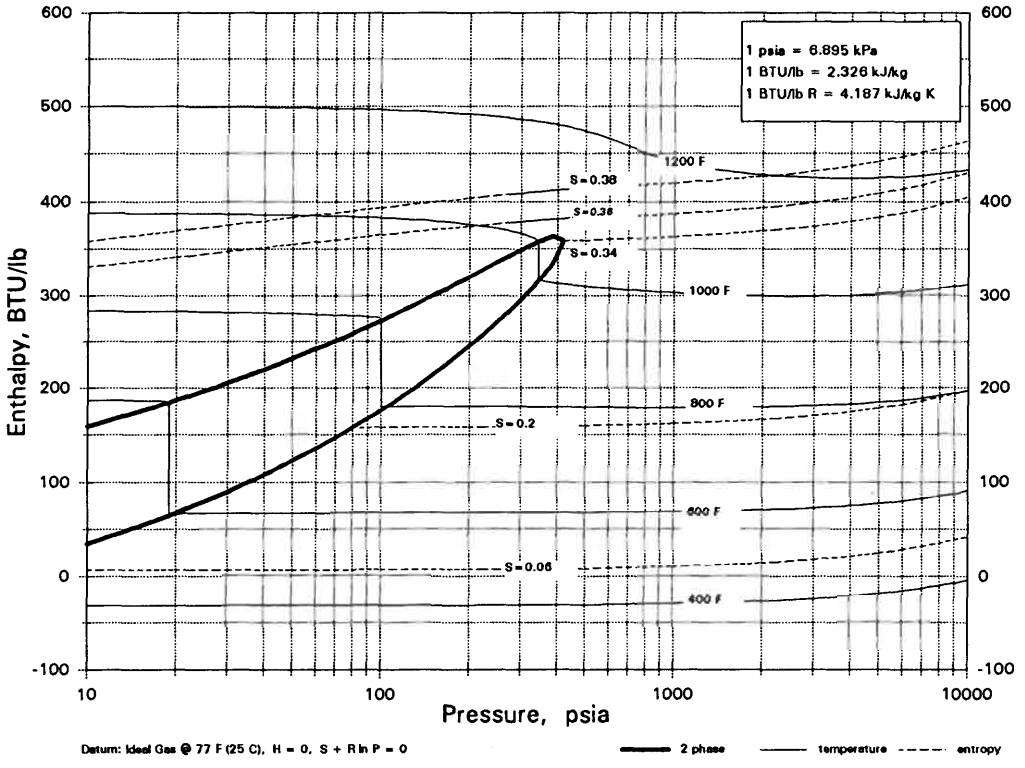
C14H10 ANTHRACENE



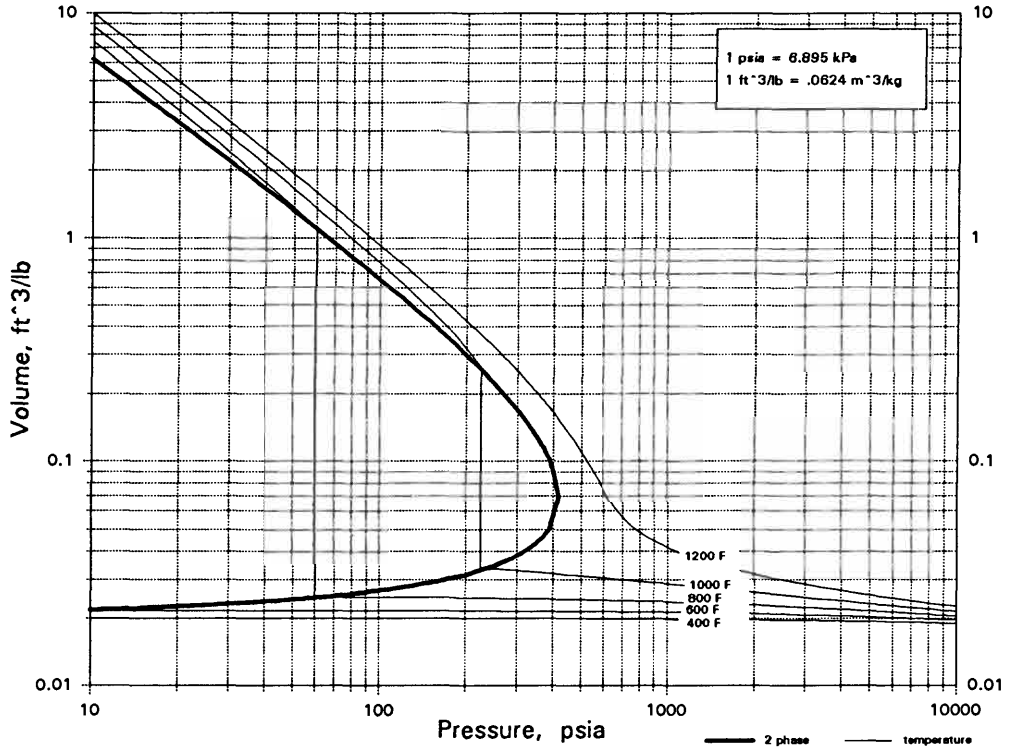


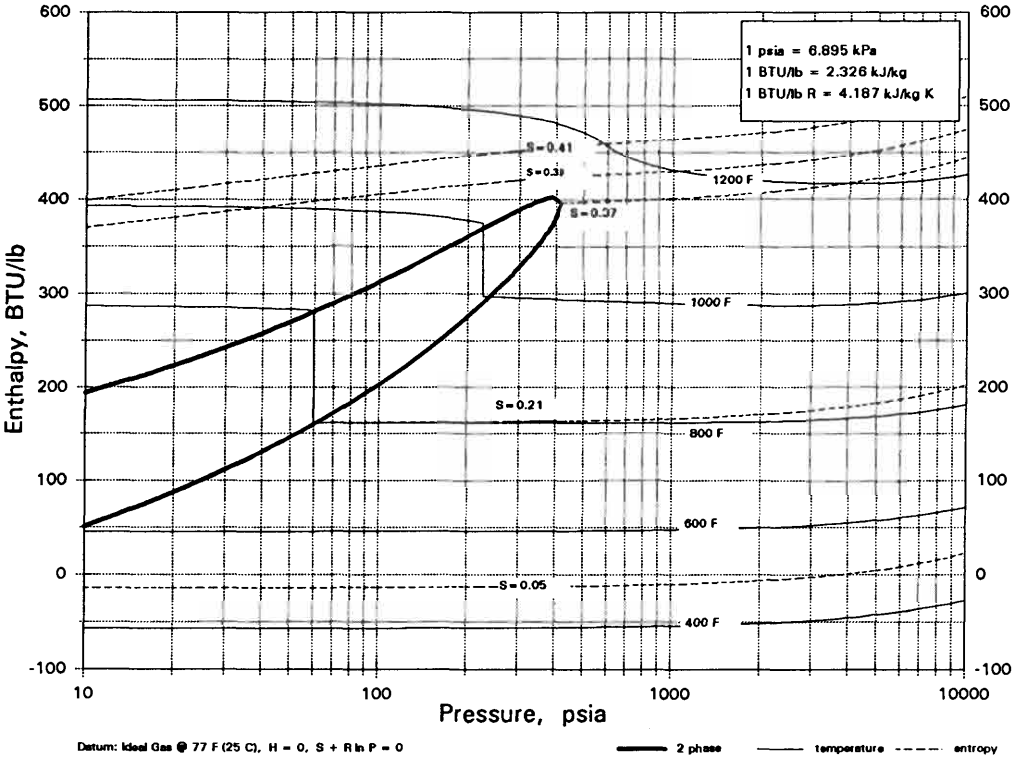
C14H10 DIPHENYLACETYLENE



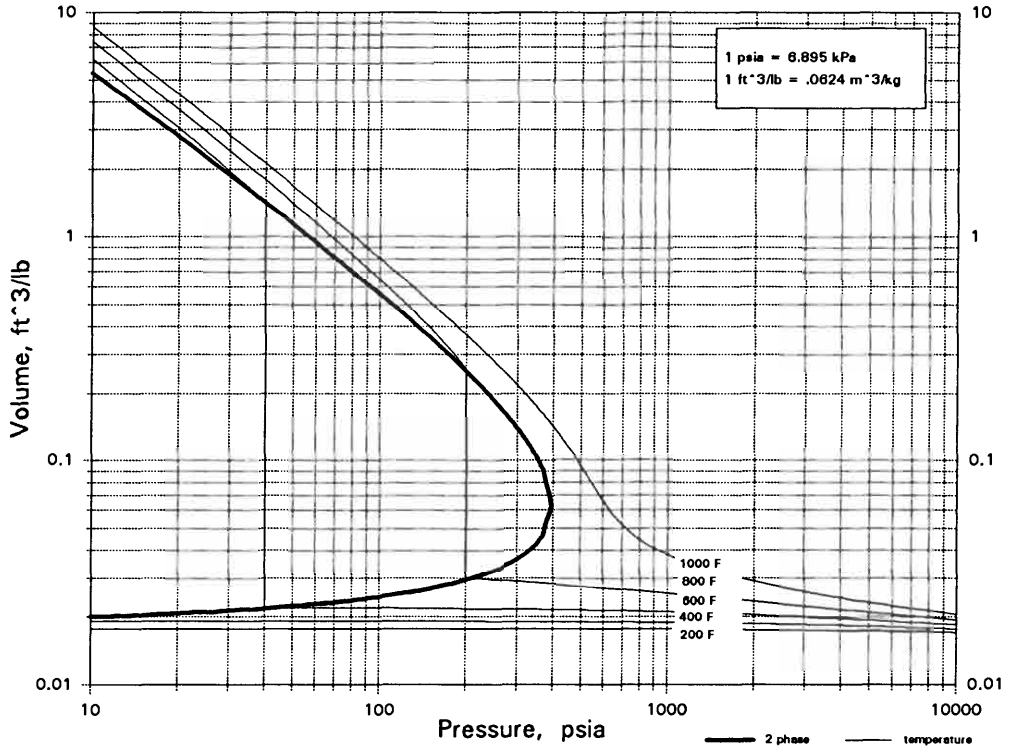


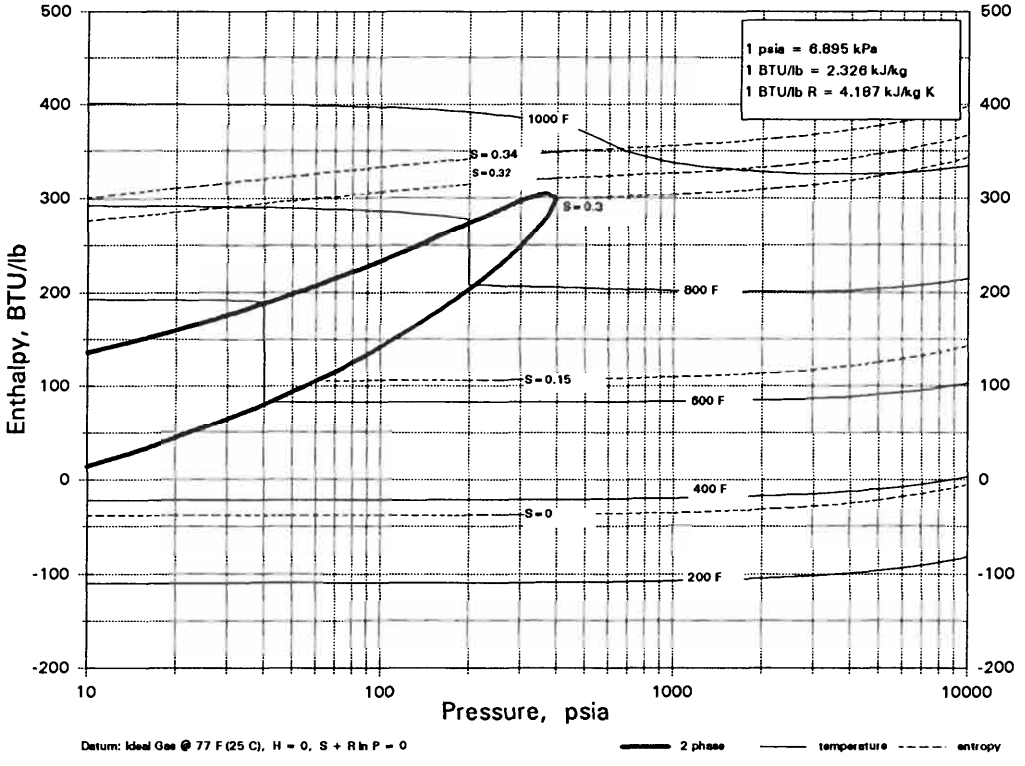
C14H10 PHENANTHRENE



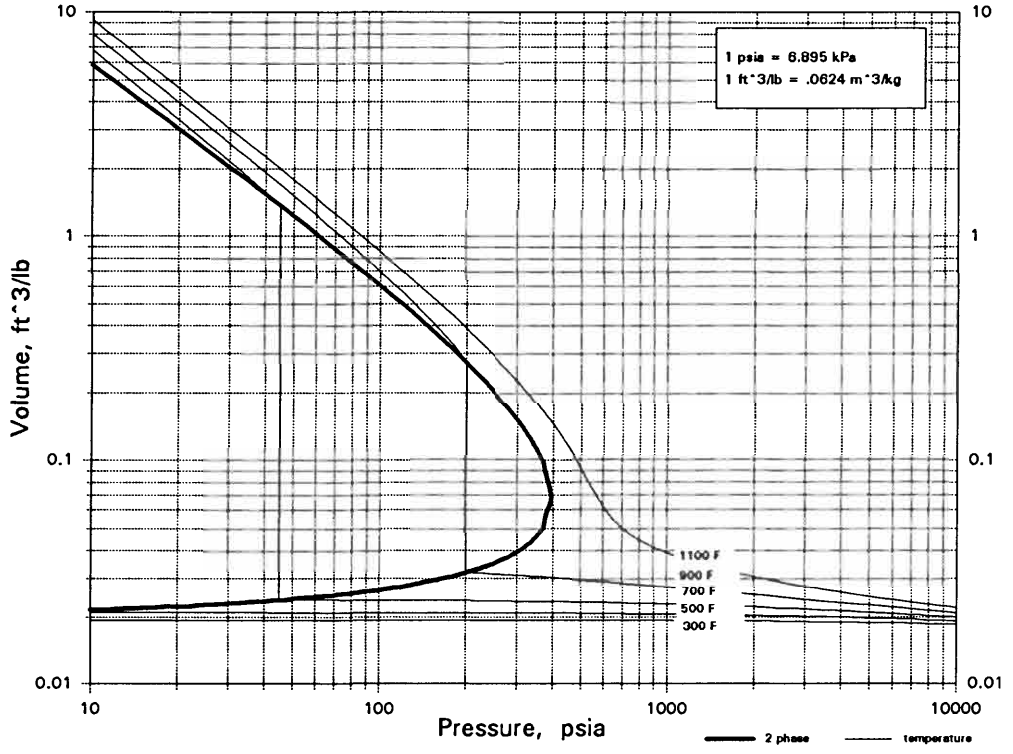


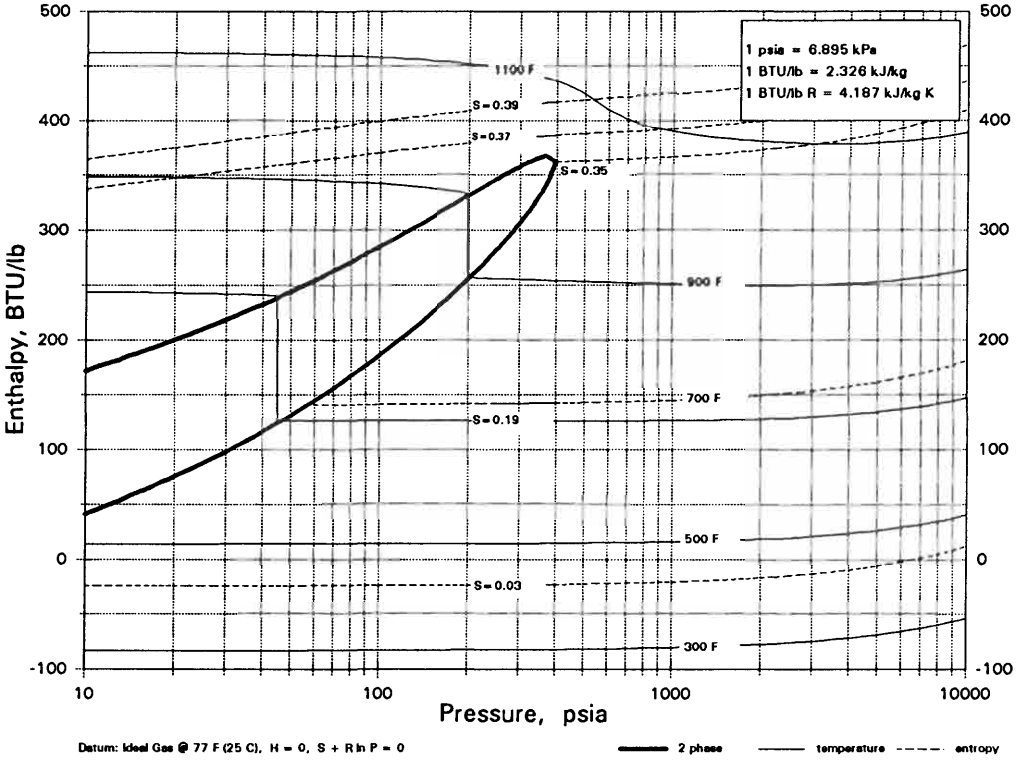
C14H12 cis-STILBENE



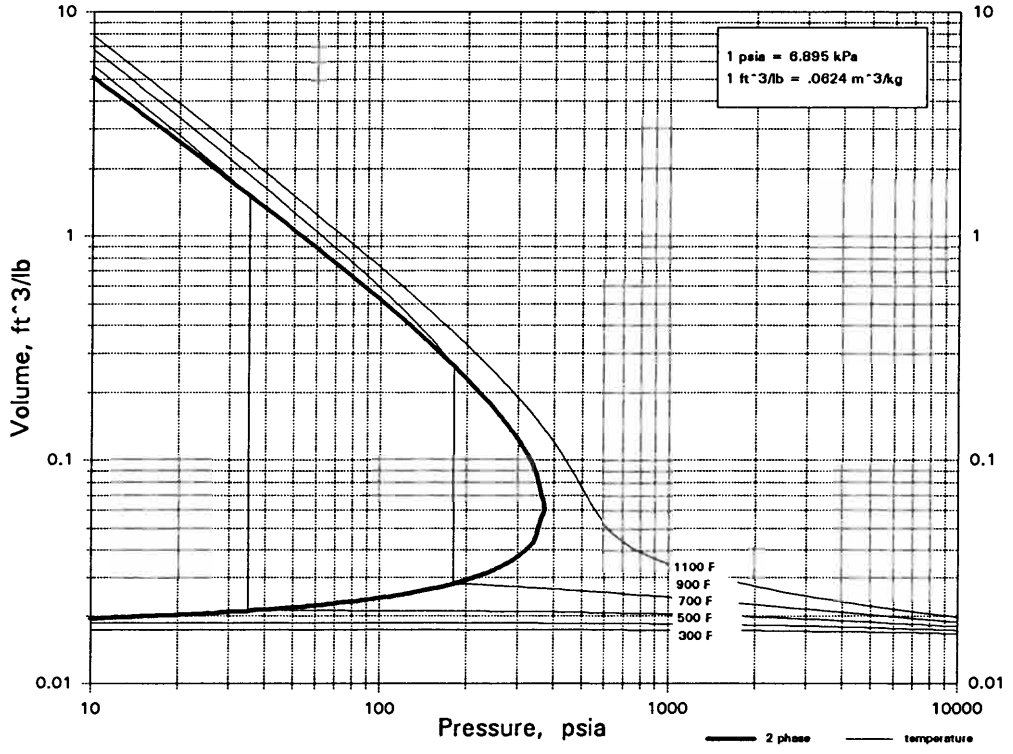


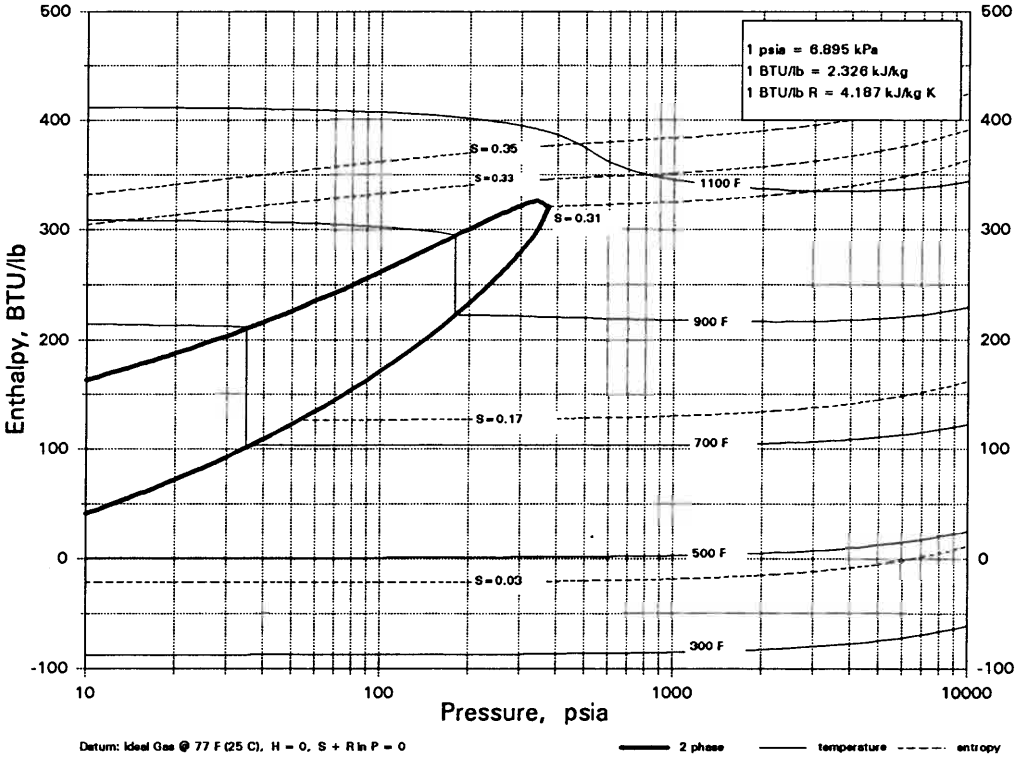
C14H12 trans-STILBENE



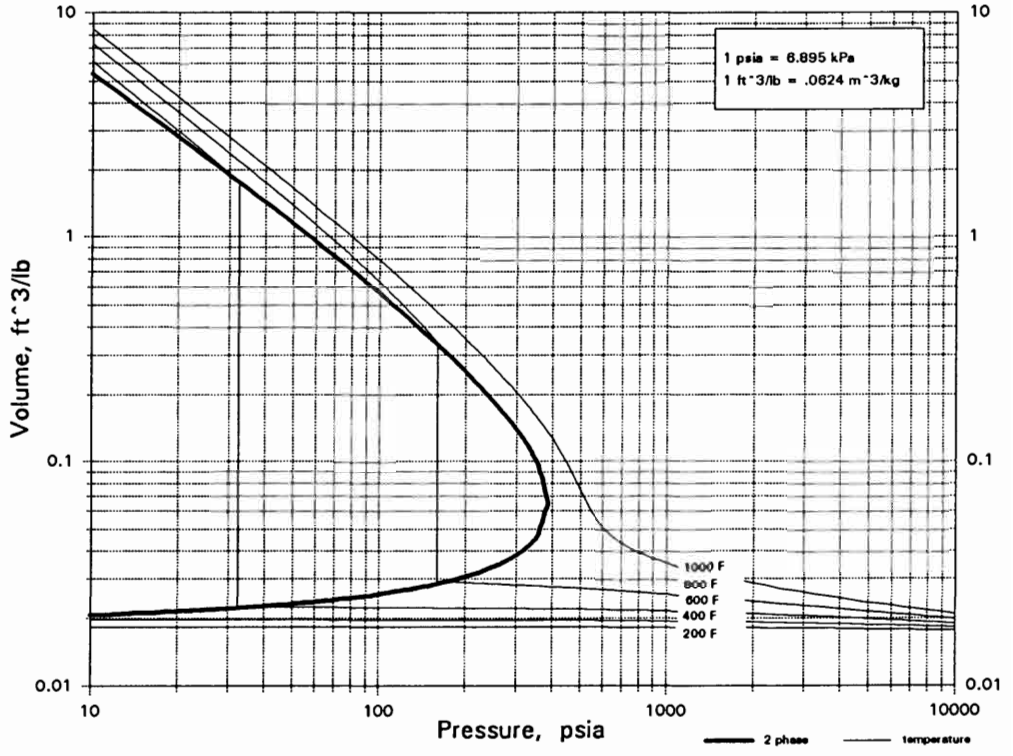


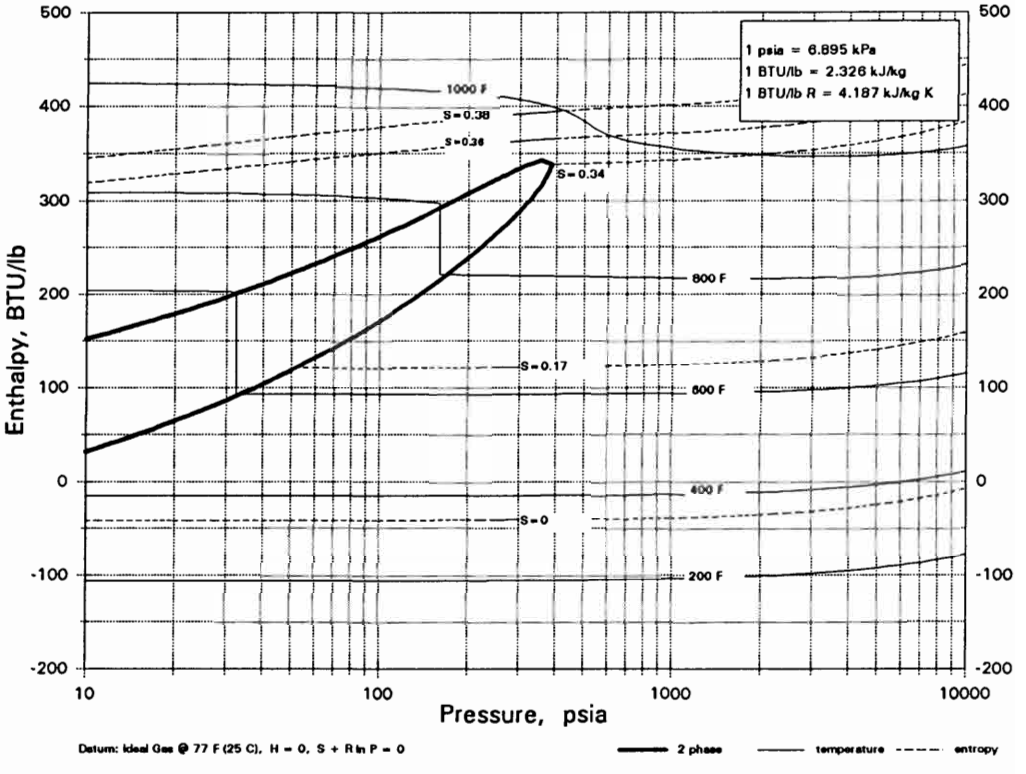
C14H12O2 BENZYL BENZOATE



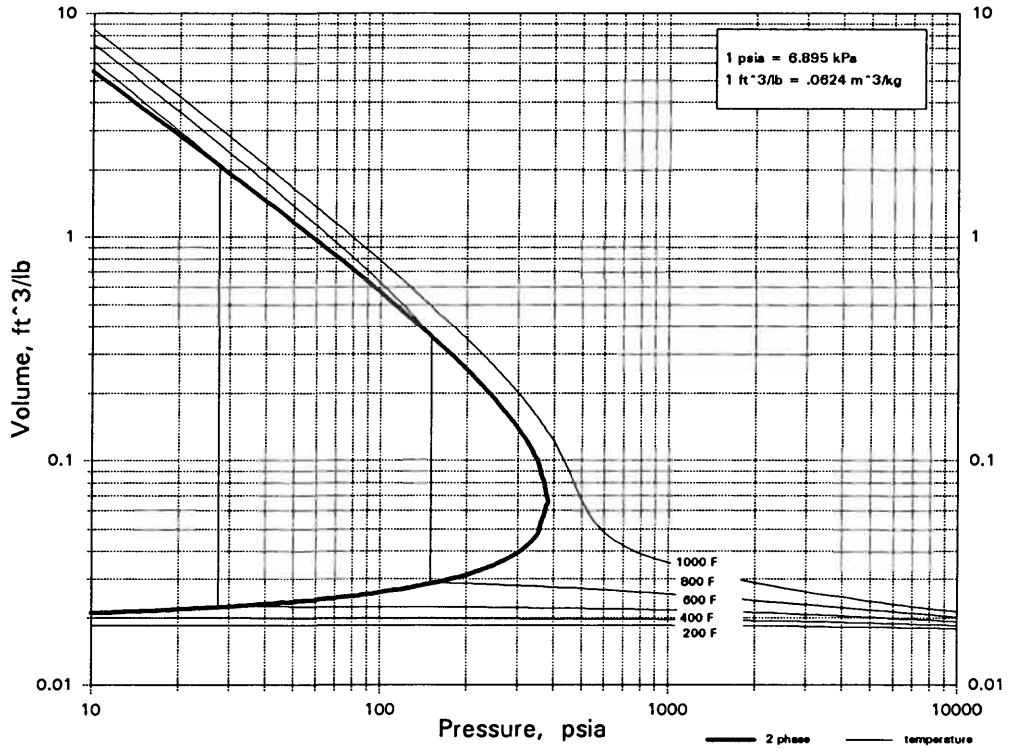


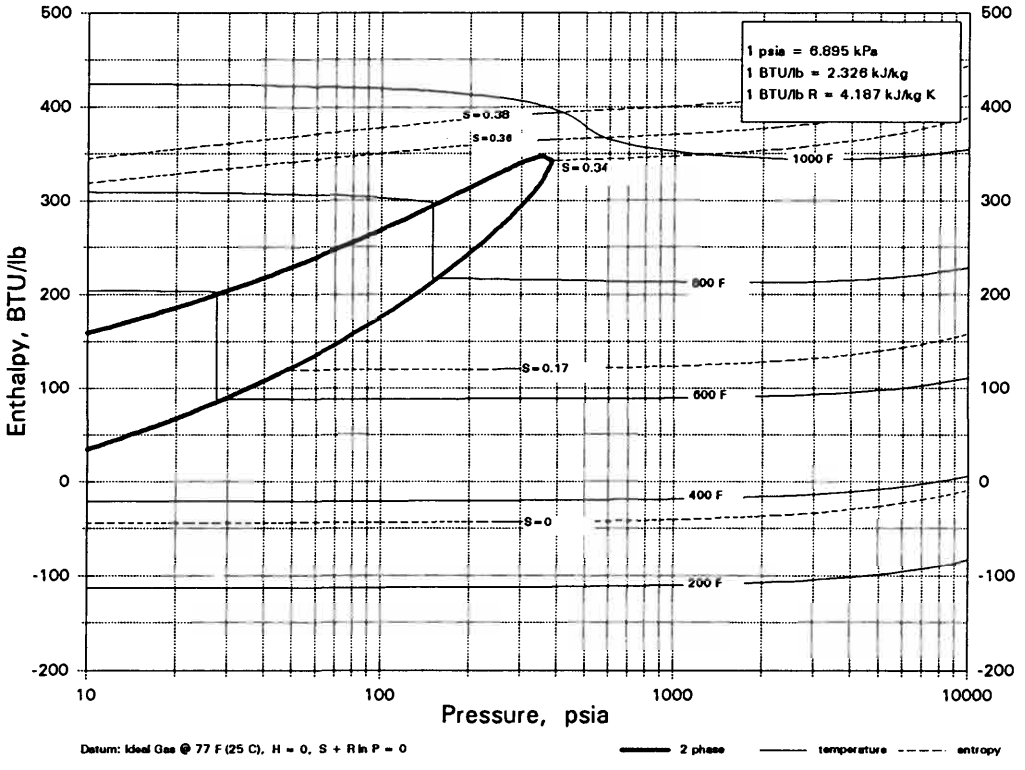
C14H14 1-1-DIPHENYLETHANE



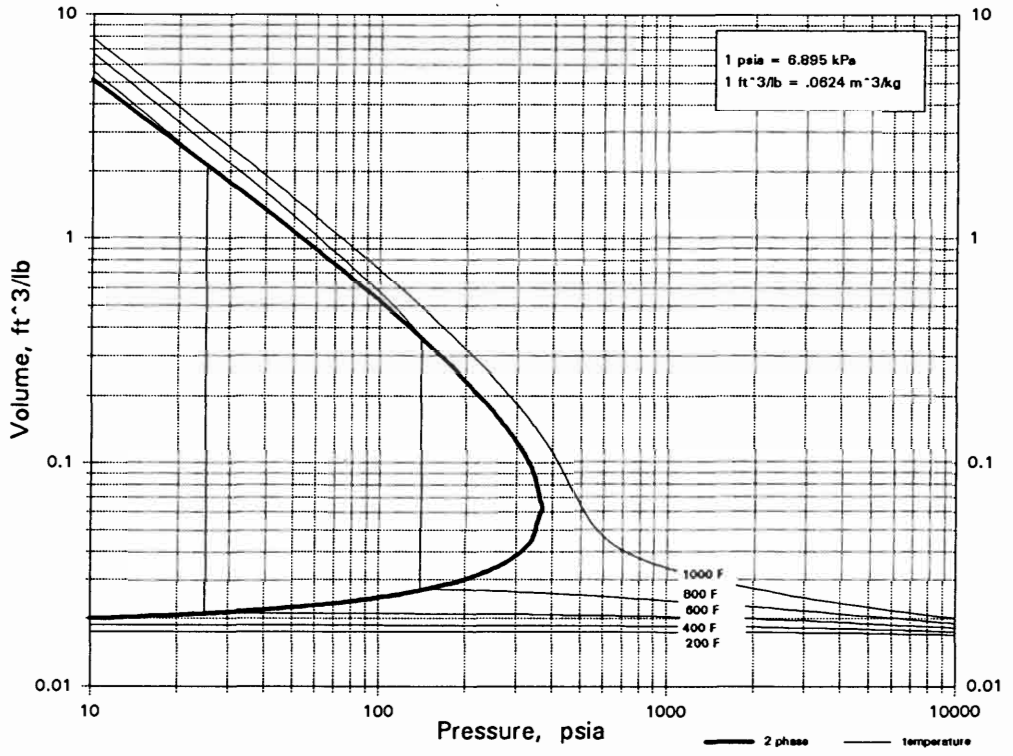


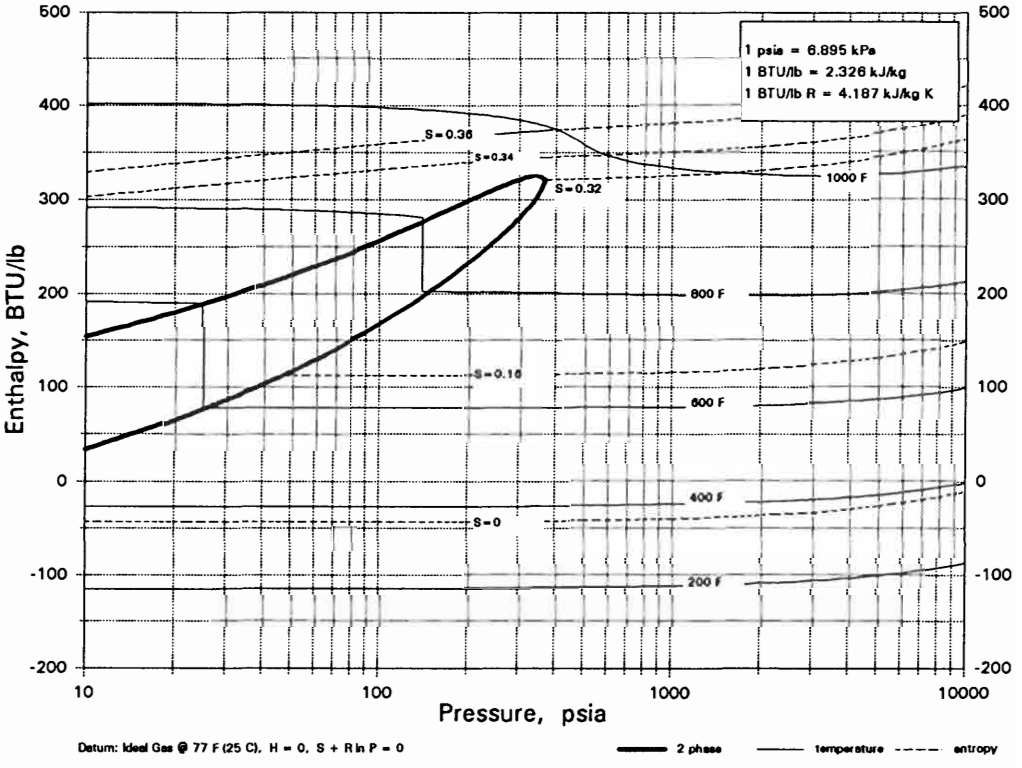
C14H14 1-2-DIPHENYLETHANE



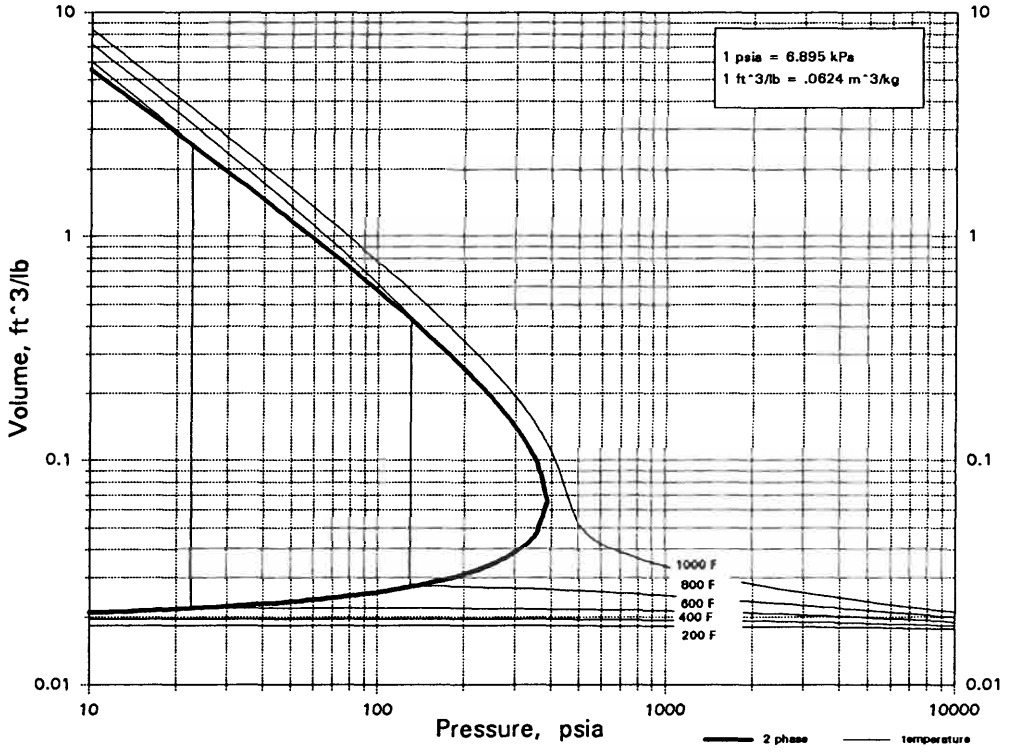


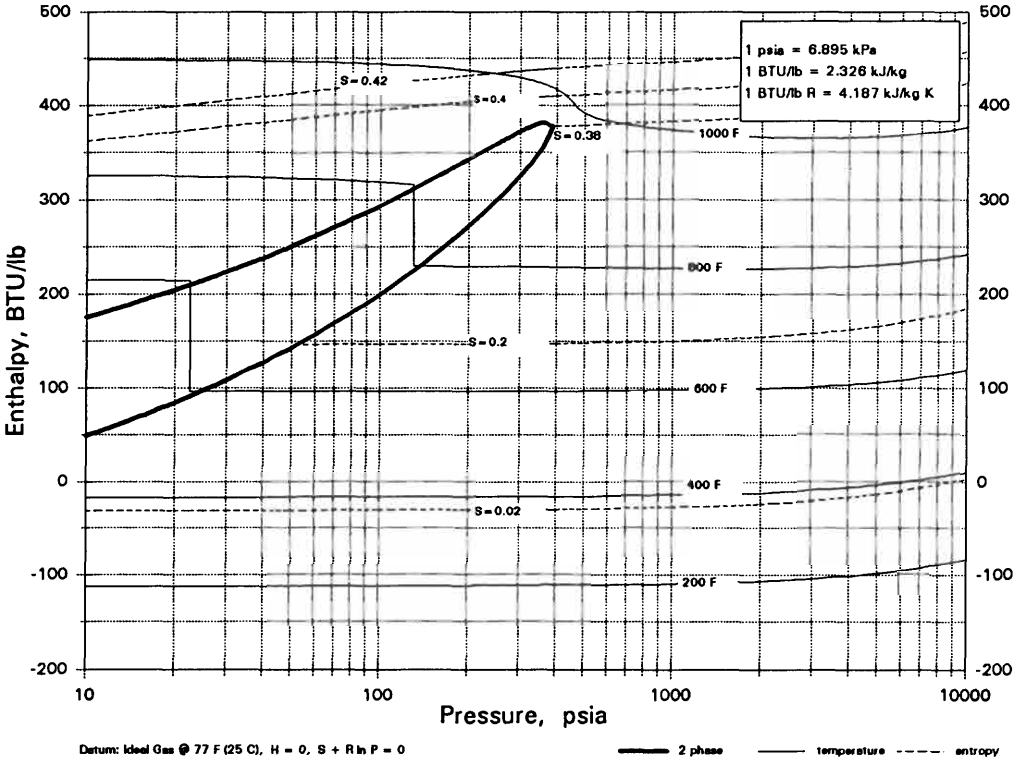
C14H14O DIBENZYL ETHER



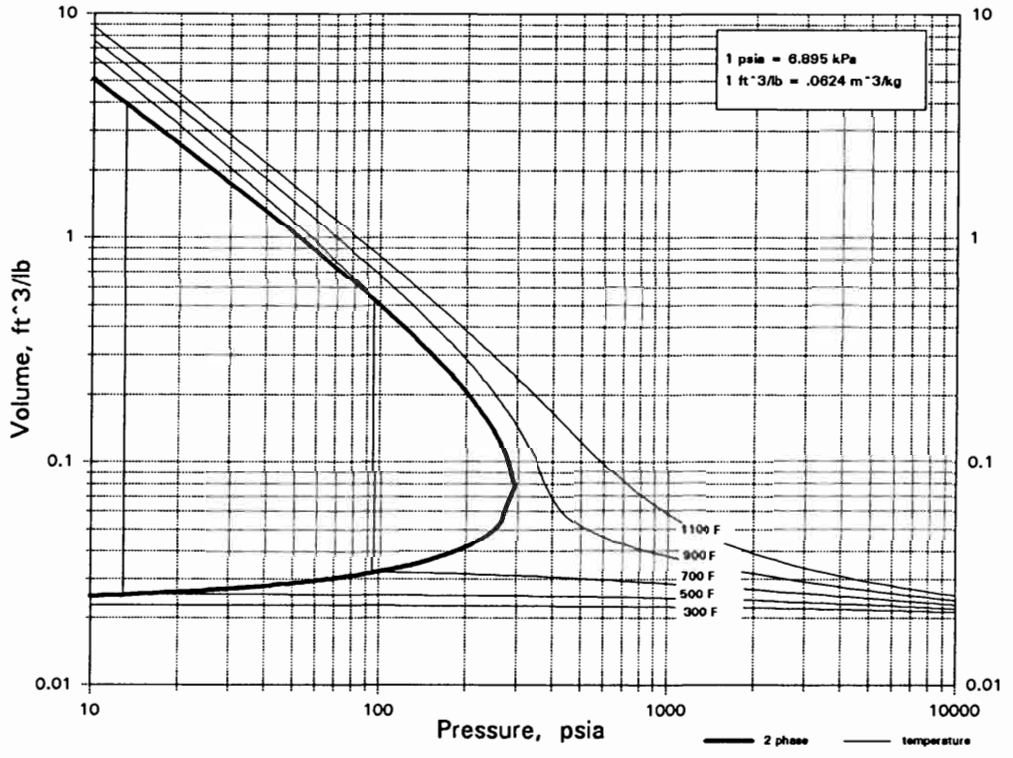


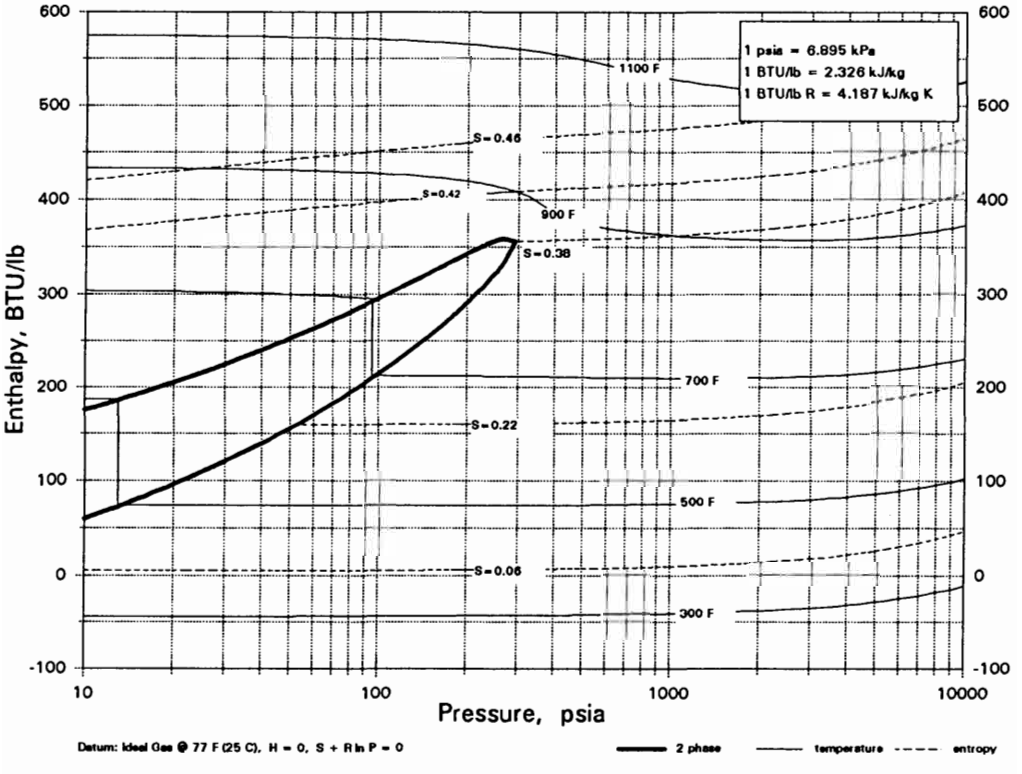
C14H16 1-n-BUTYLNAPHTHALENE



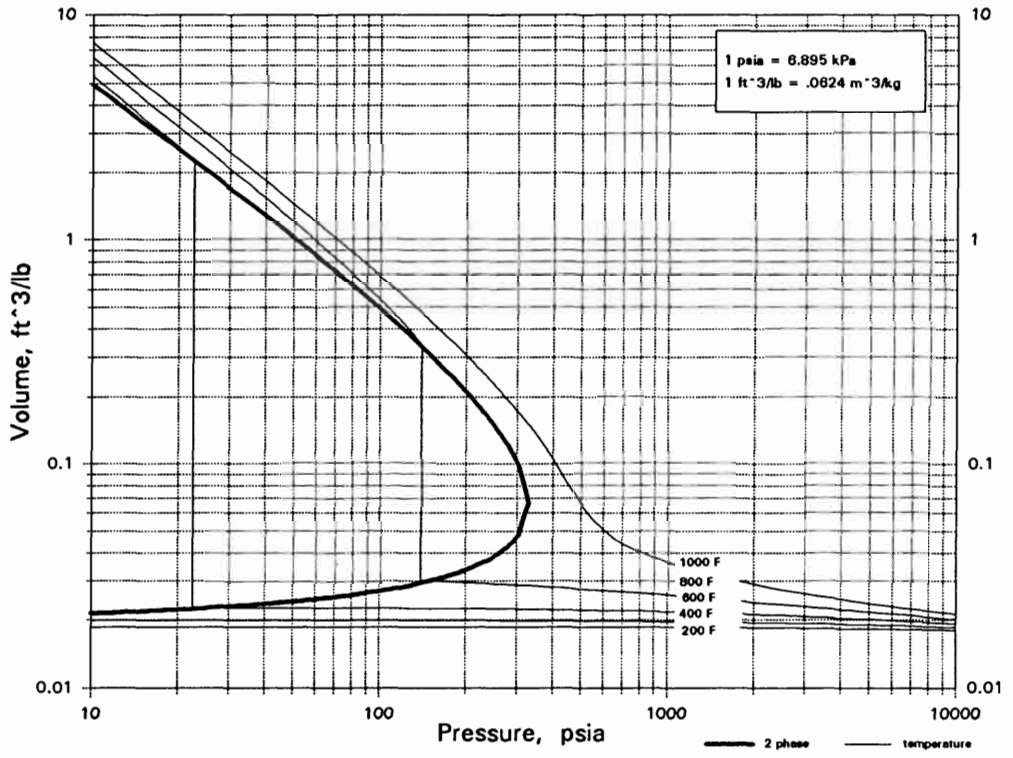


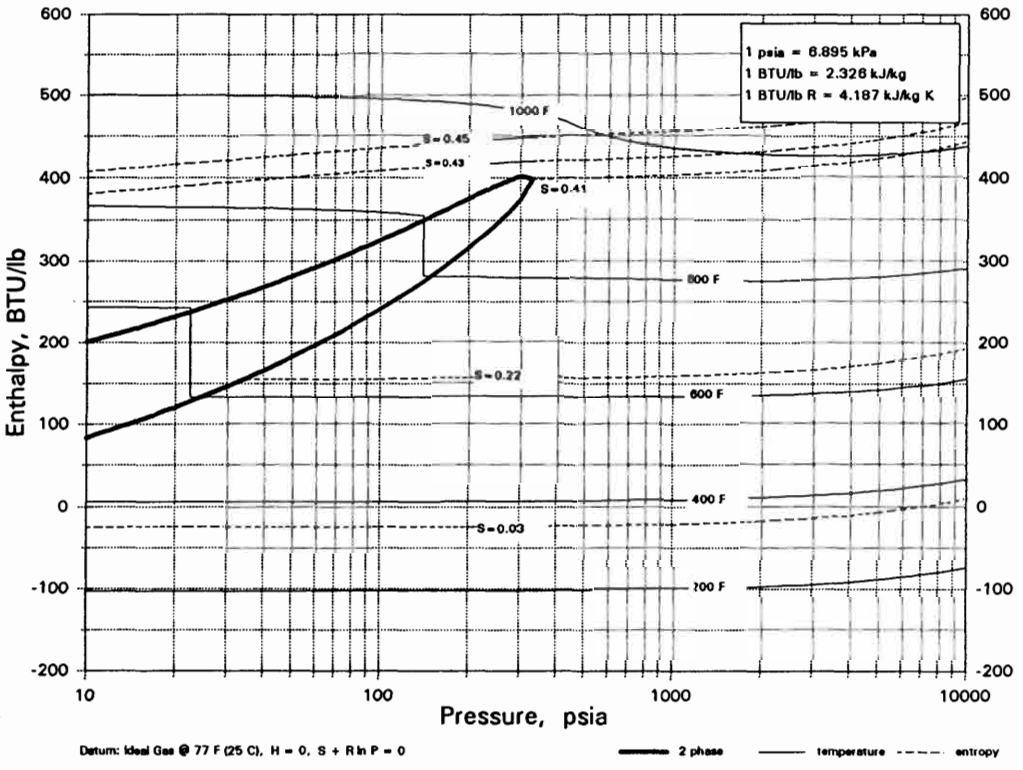
C14H22 n-OCTYLBENZENE



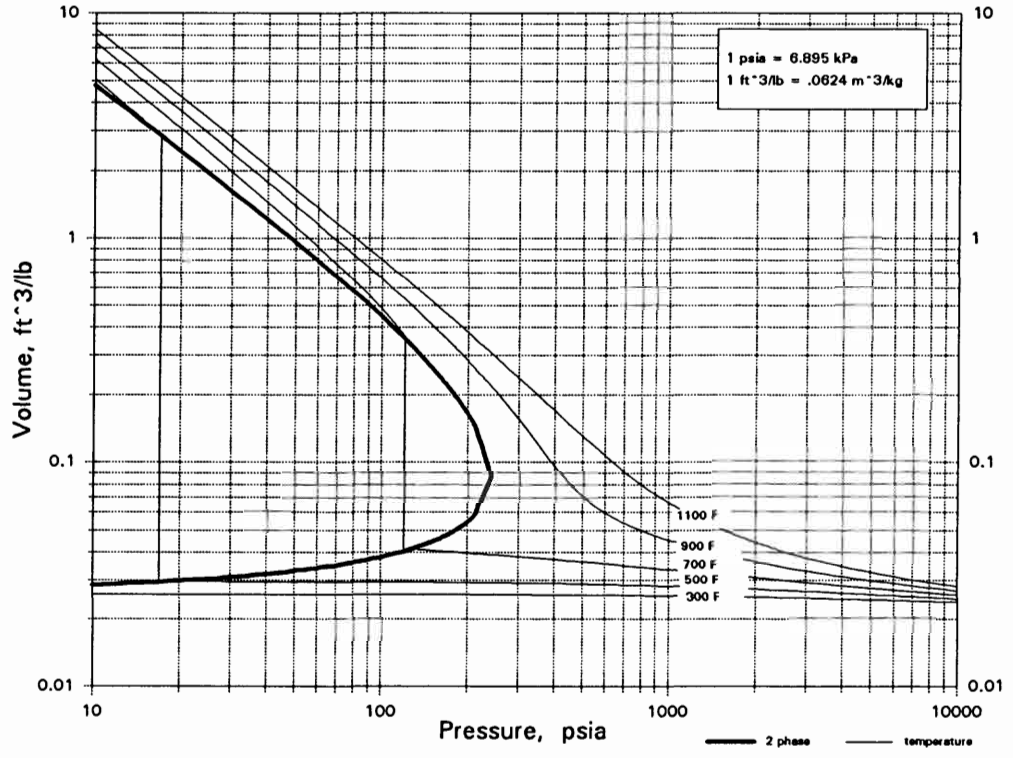


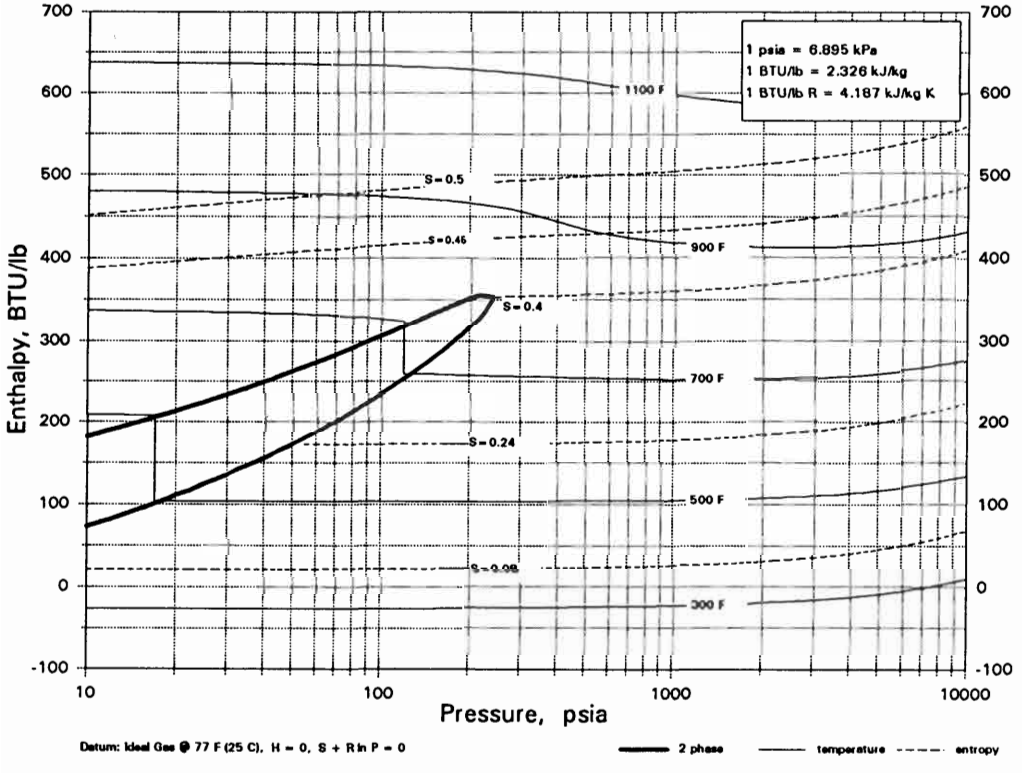
C14H22O p-tert-OCTYLPHENOL



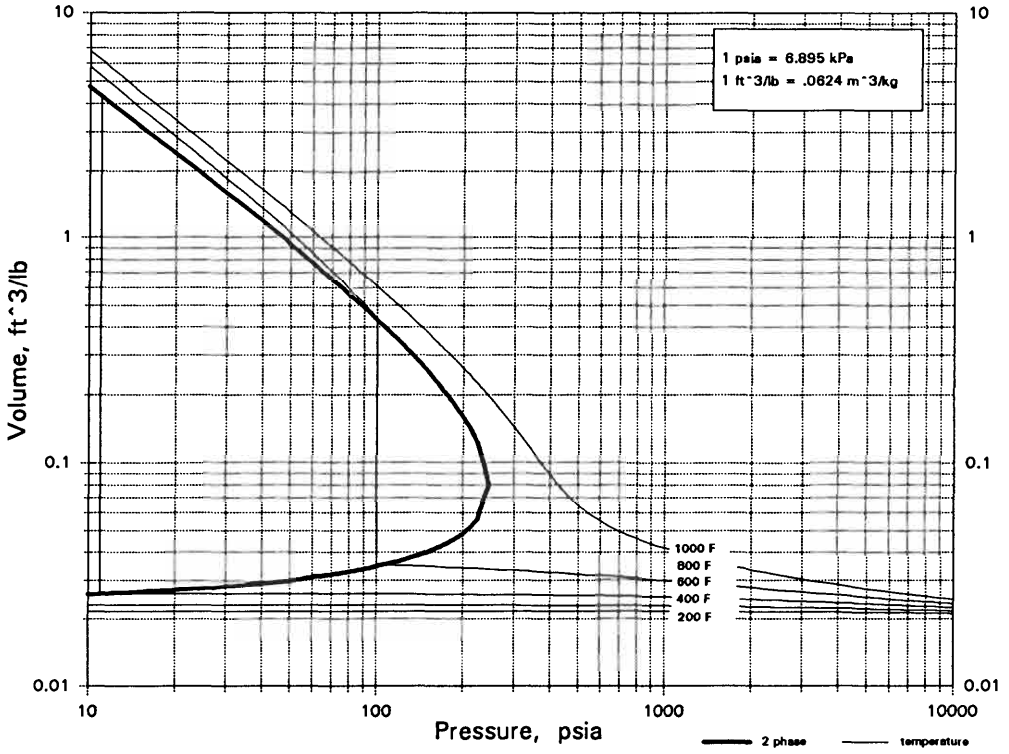


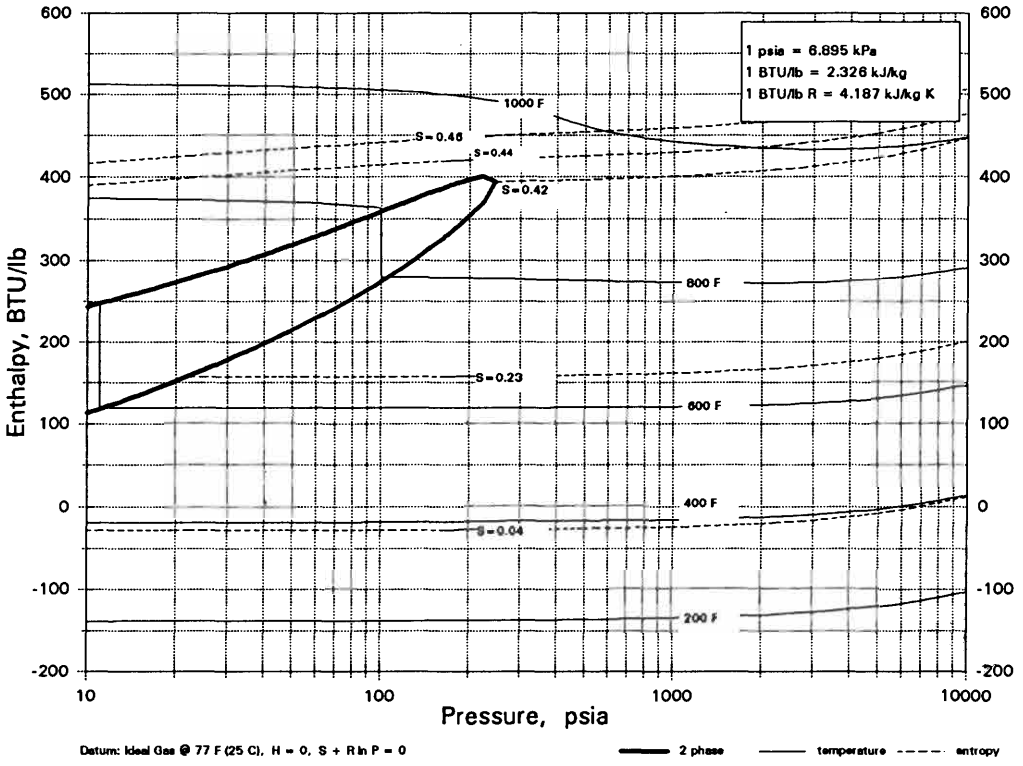
C14H28 1-TETRADECENE



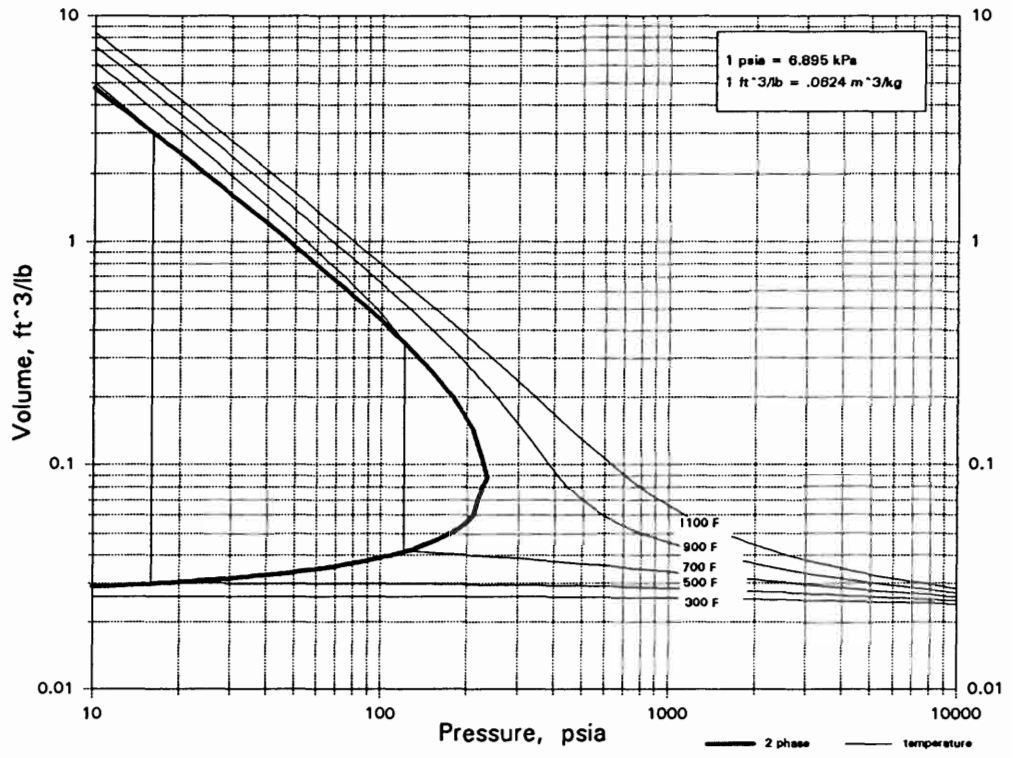


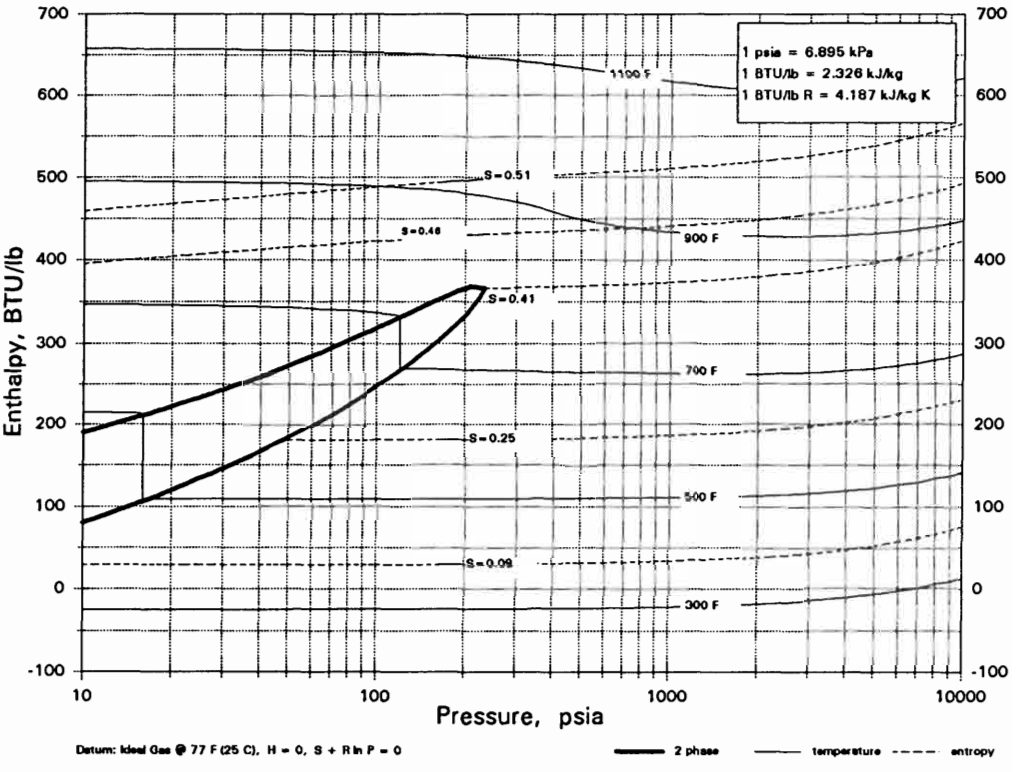
C14H28O2 n-TETRADECANOIC ACID



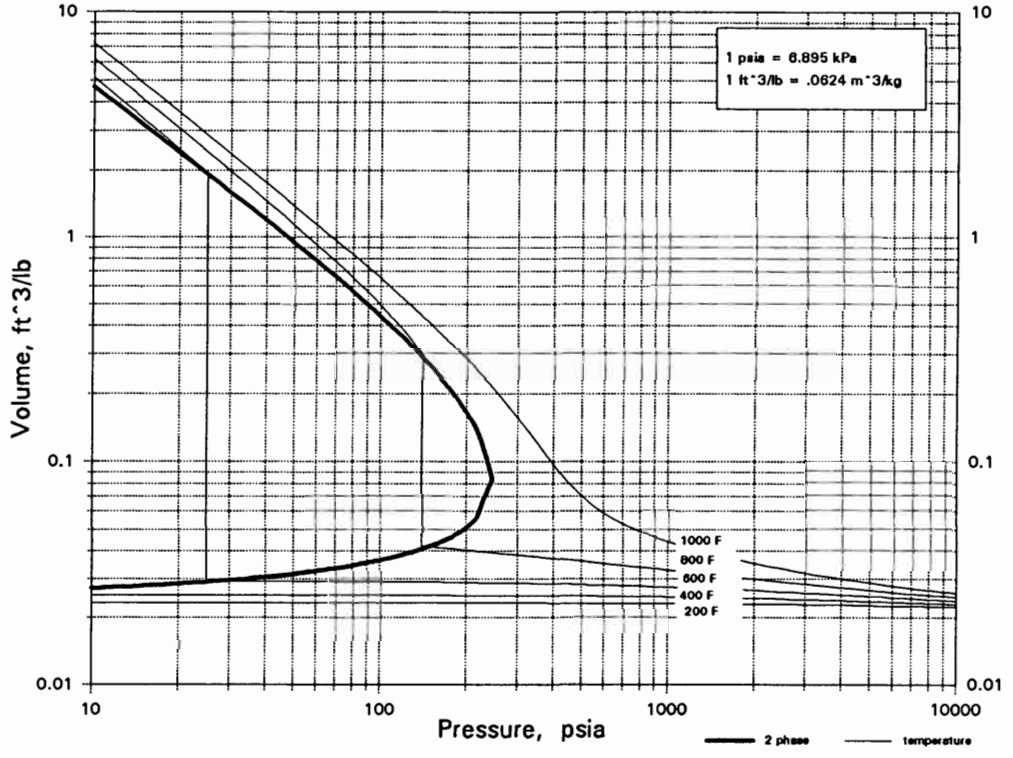


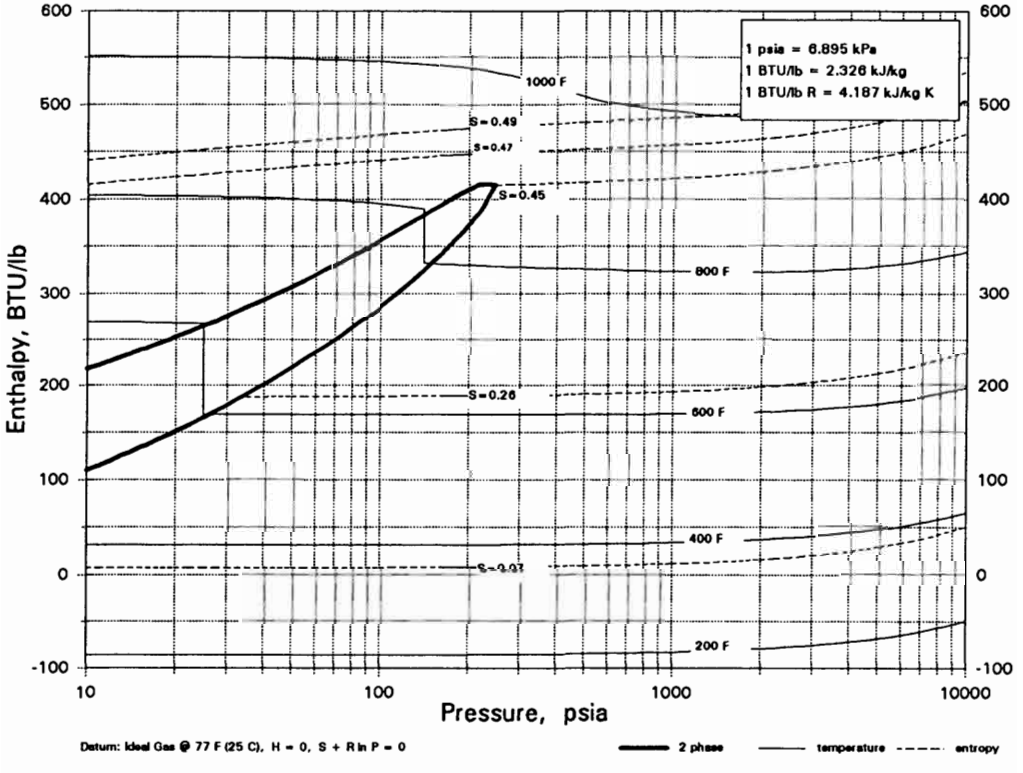
C14H30 n-TETRADECANE



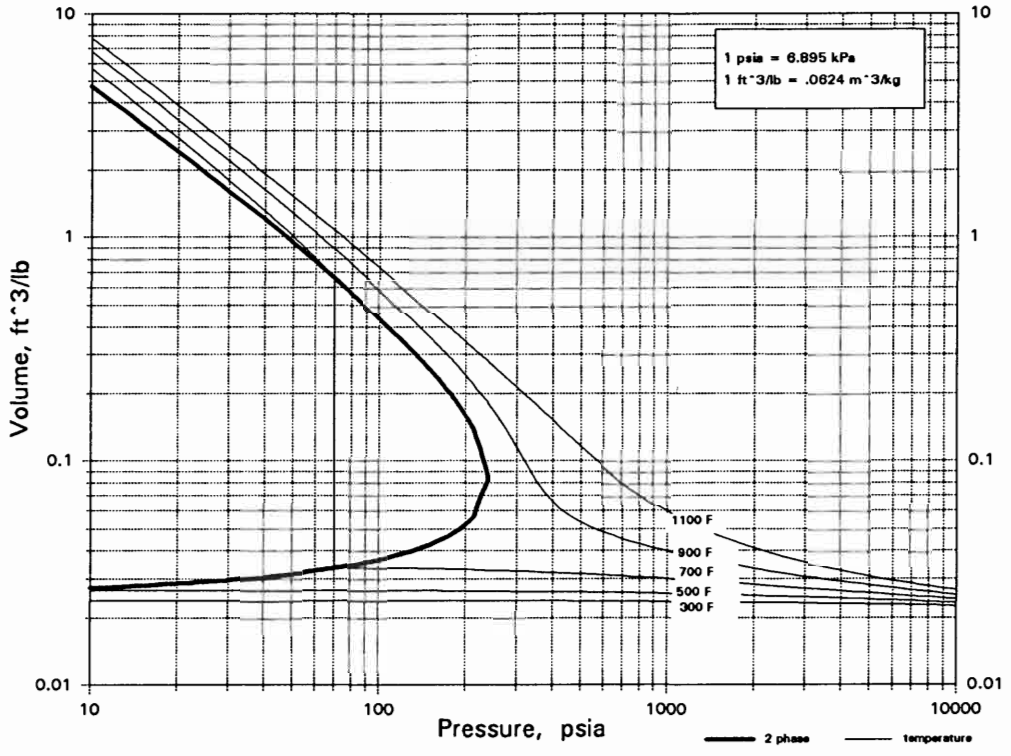


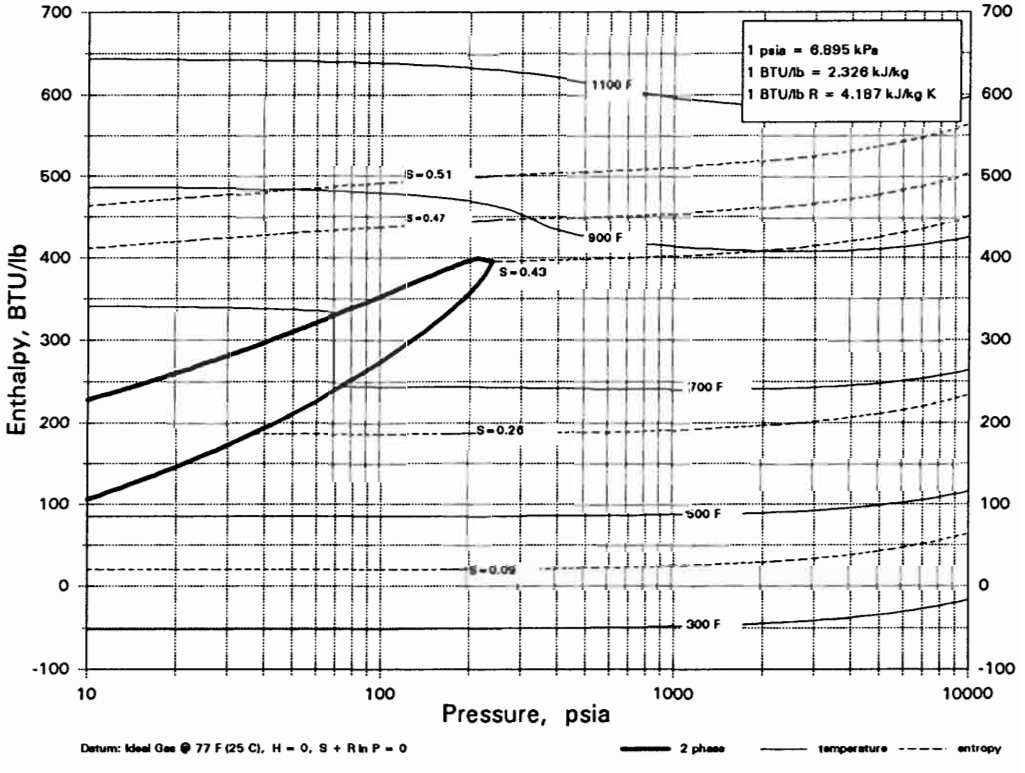
C14H30O 1-TETRADECANOL



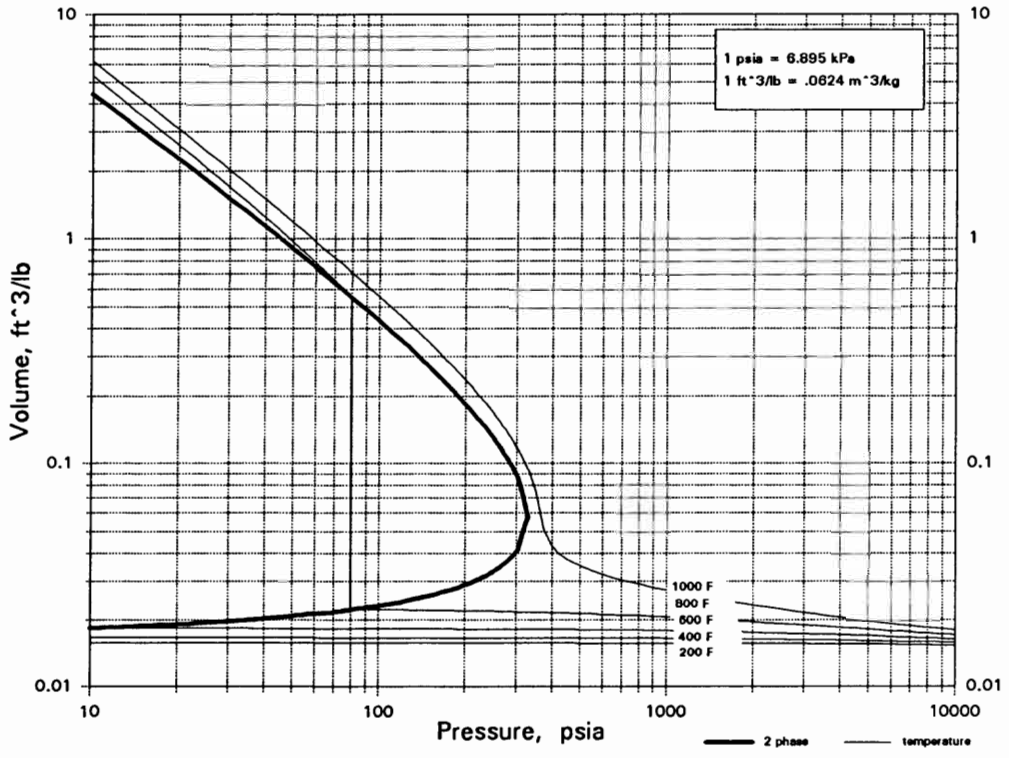


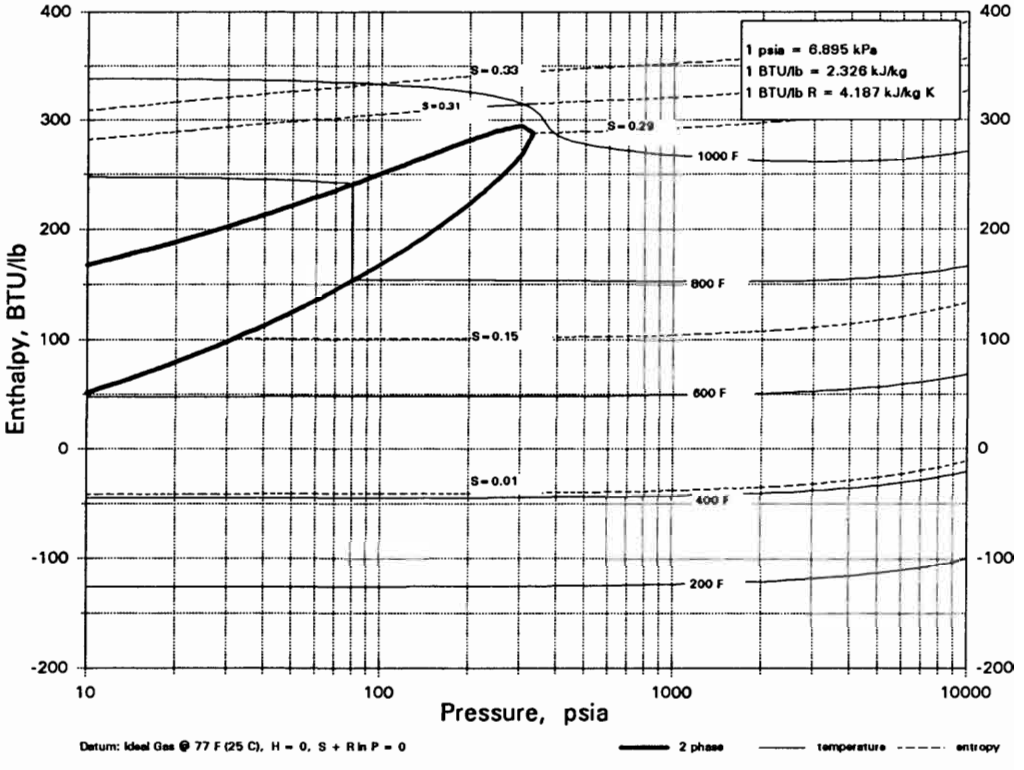
C14H31N TETRADECYLAMINE



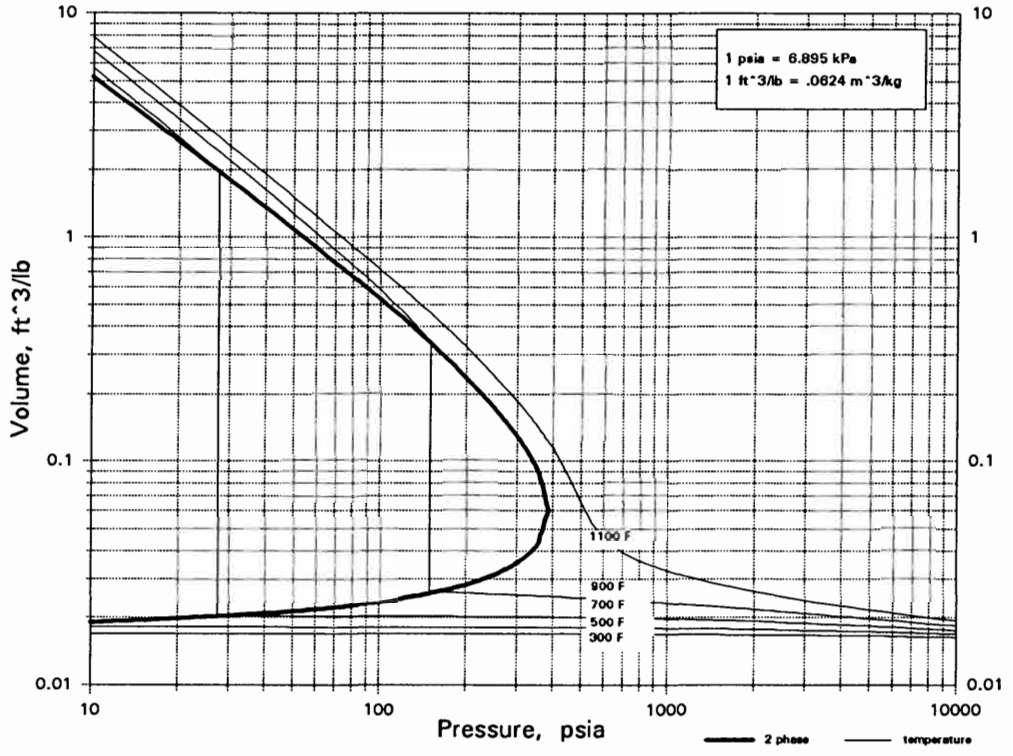


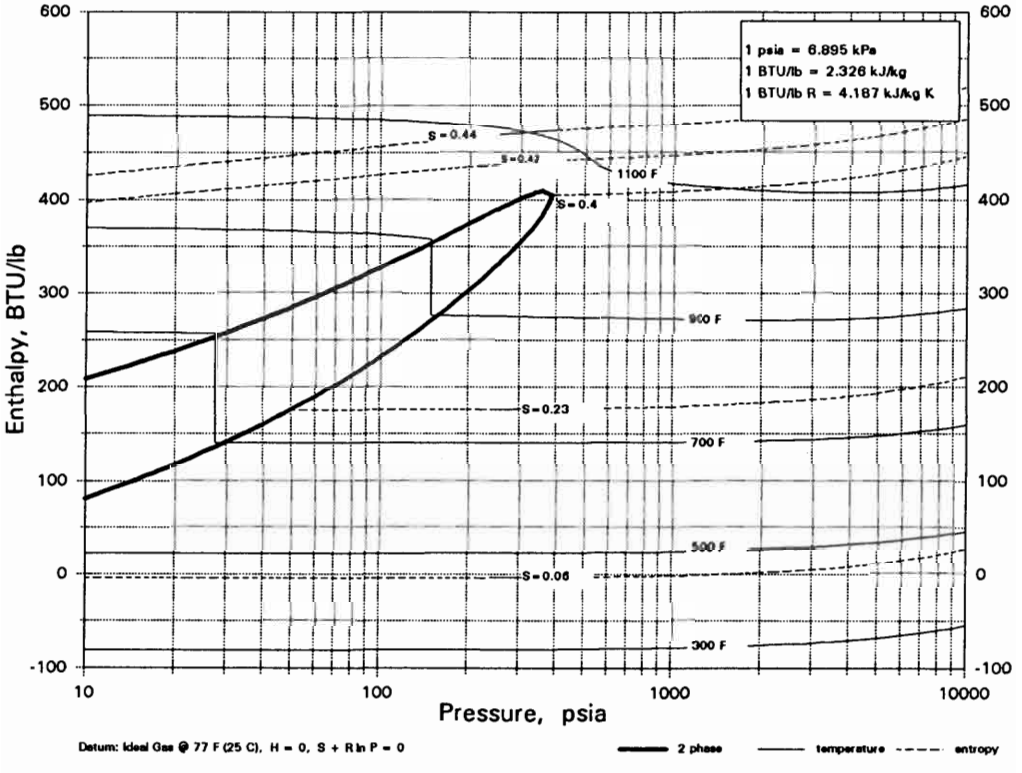
C15H10N2O2 DIPHENYLMETHANE-4-4'-DIISOCYANATE



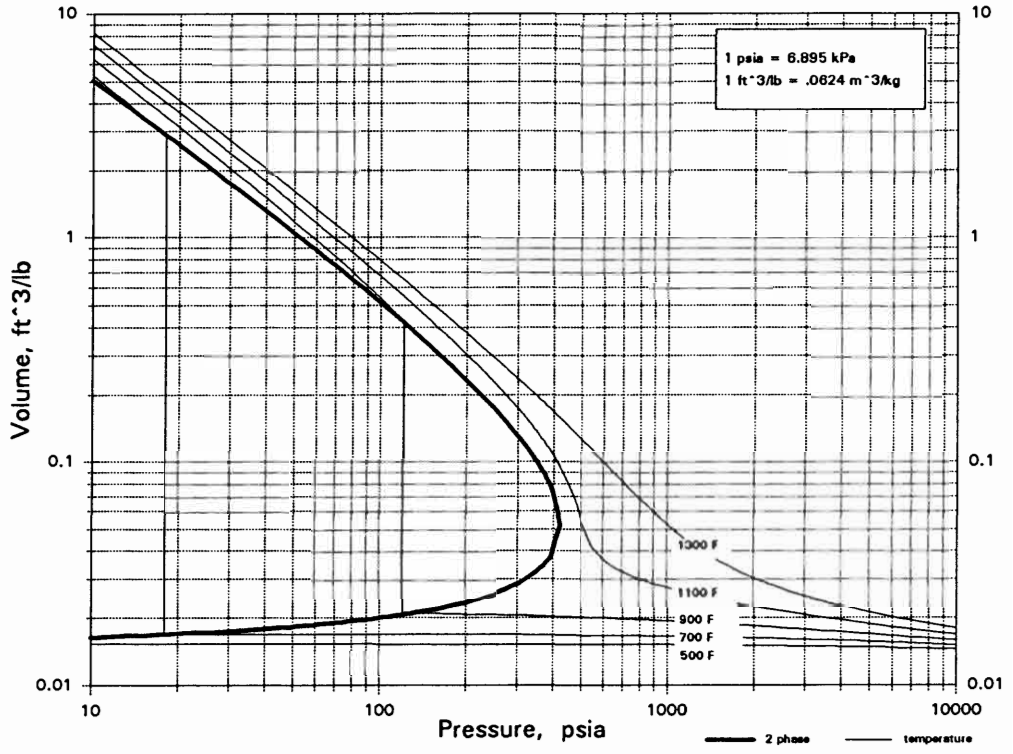


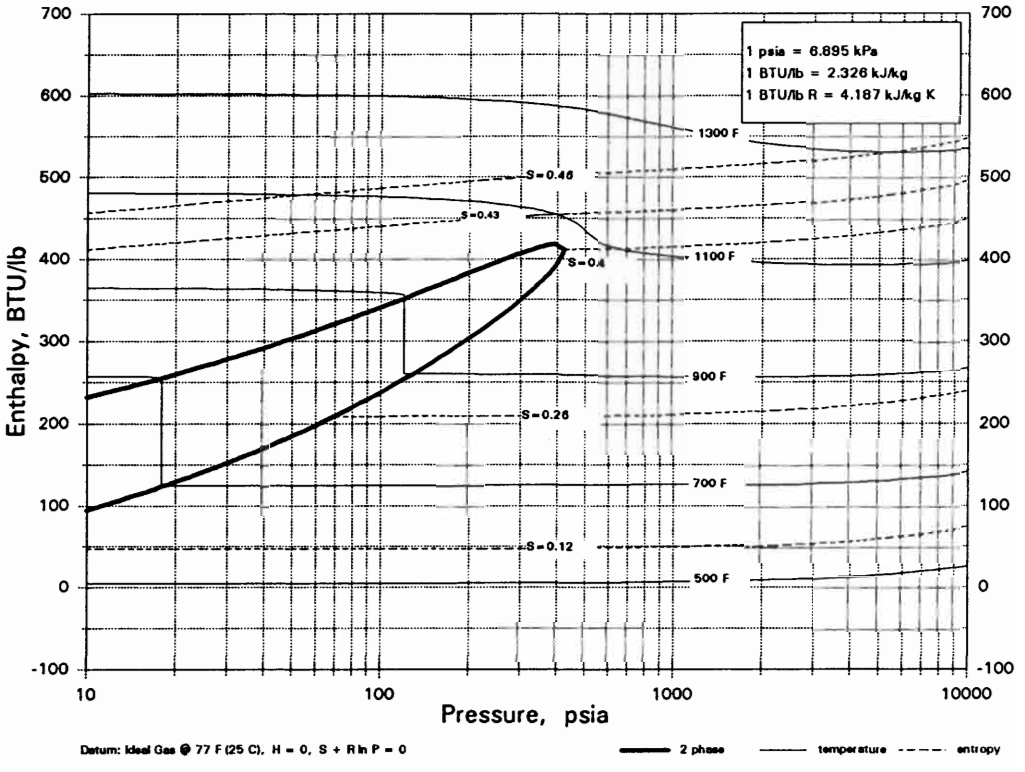
C15H16O p-CUMYLPHENOL



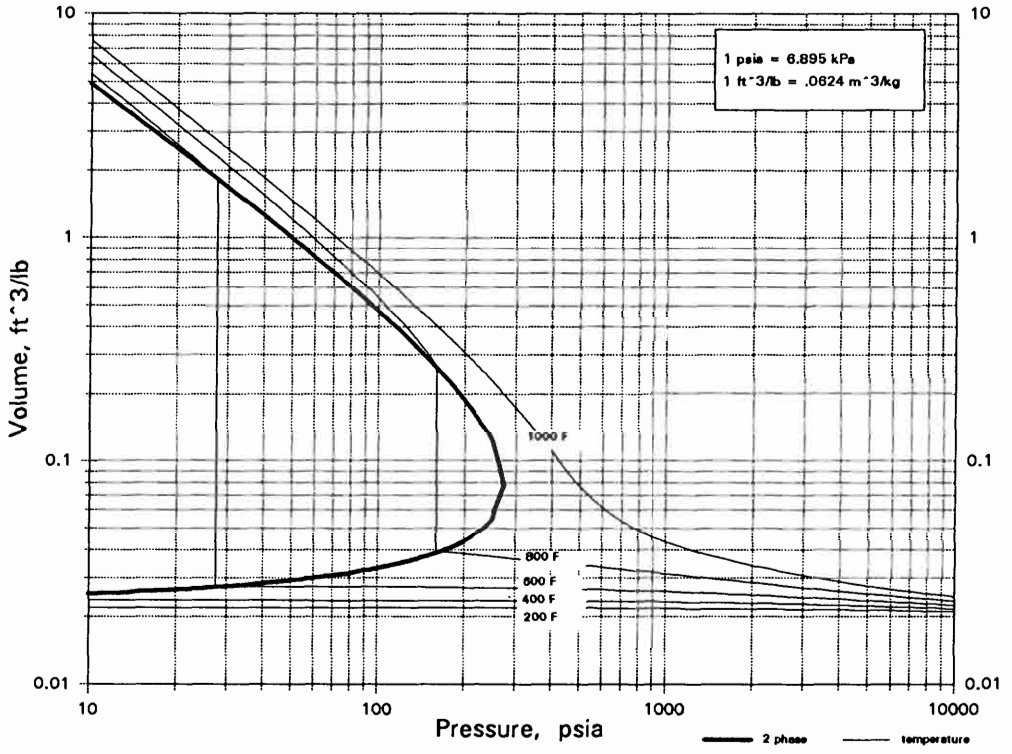


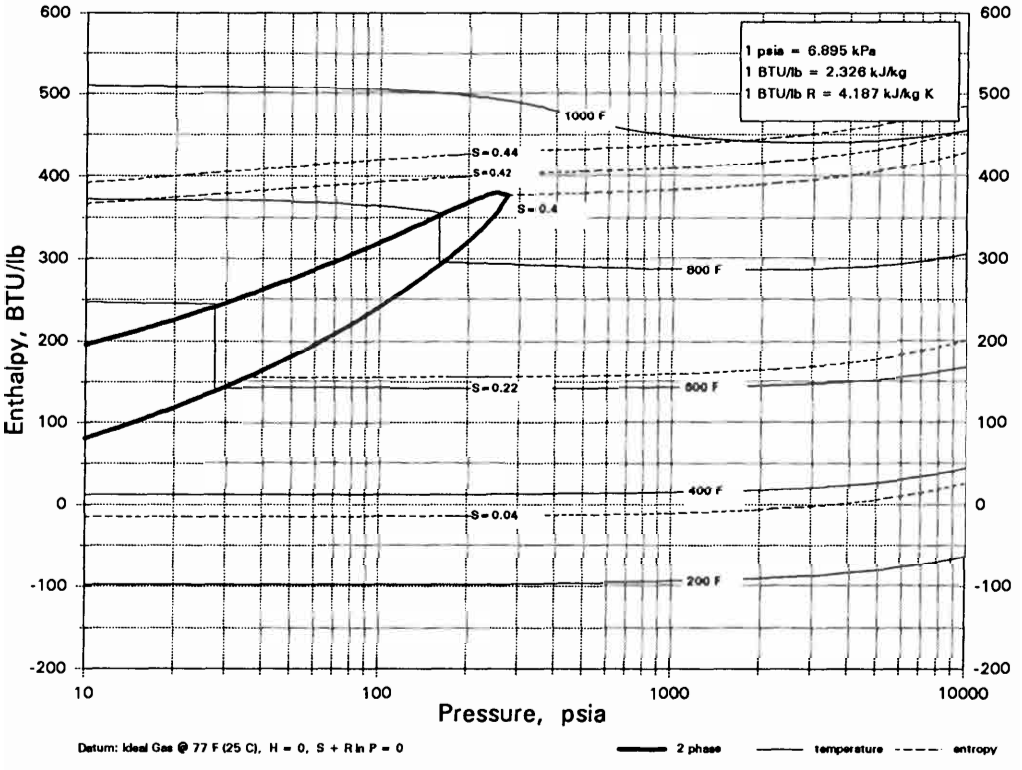
C15H16O2 BISPHENOL A



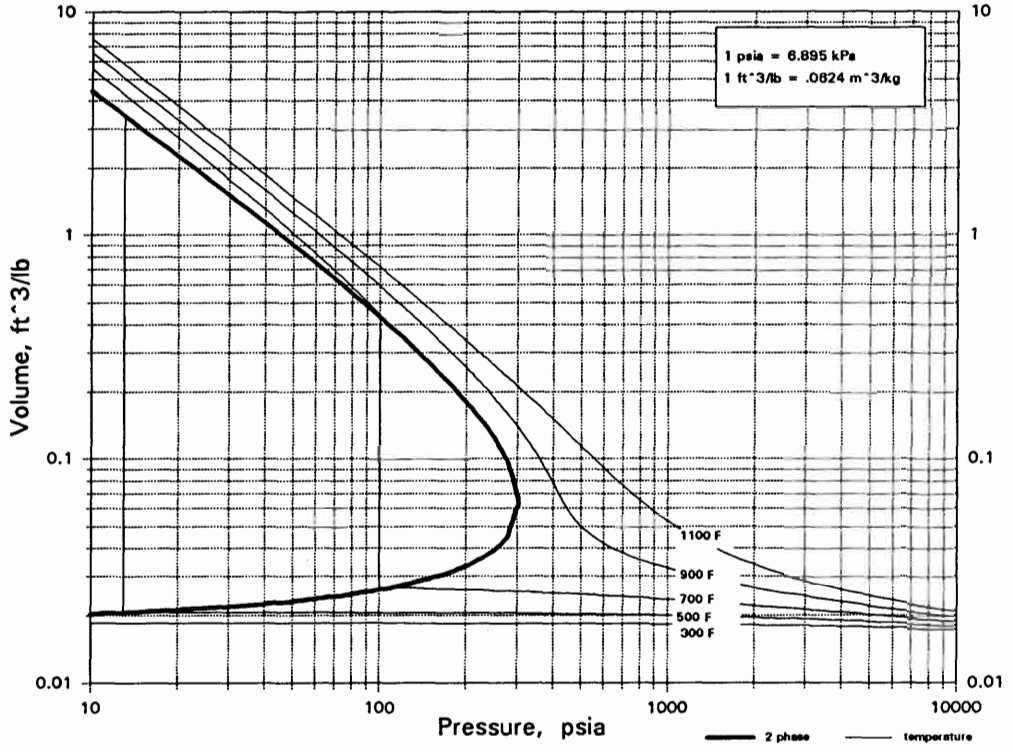


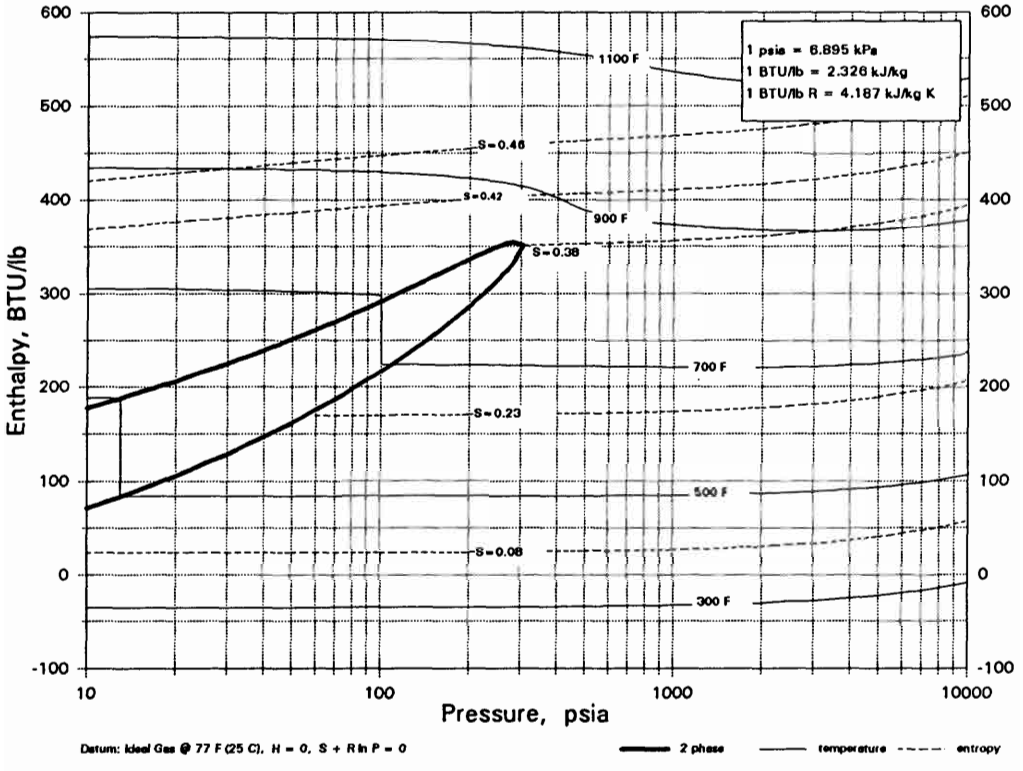
C15H24 n-NONYLBENZENE



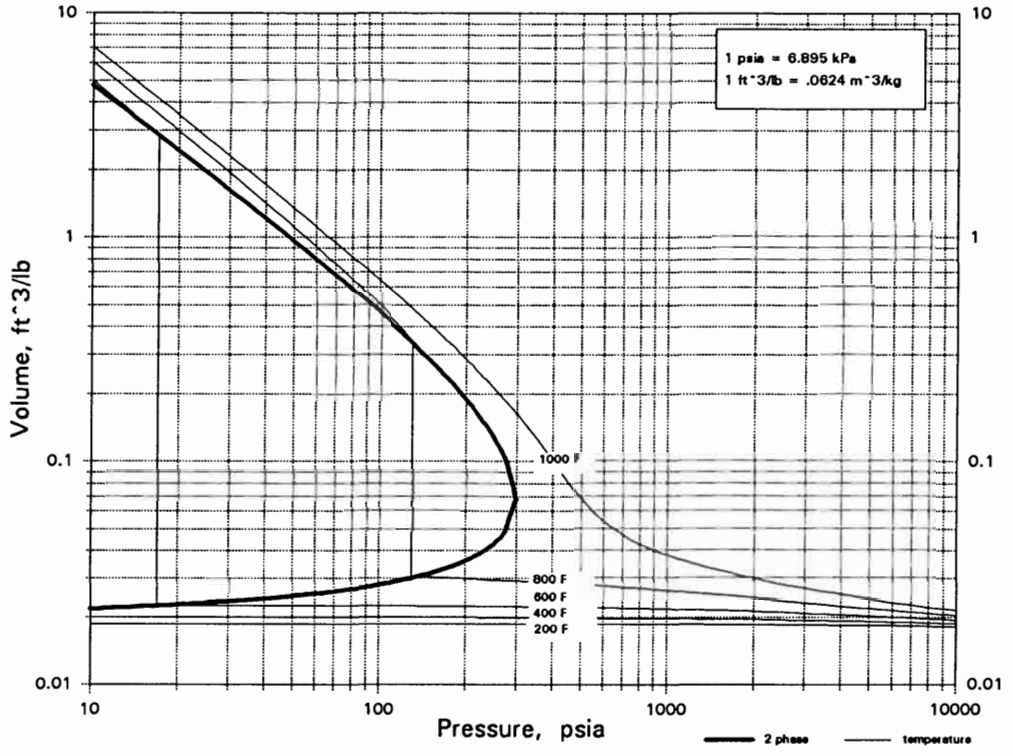


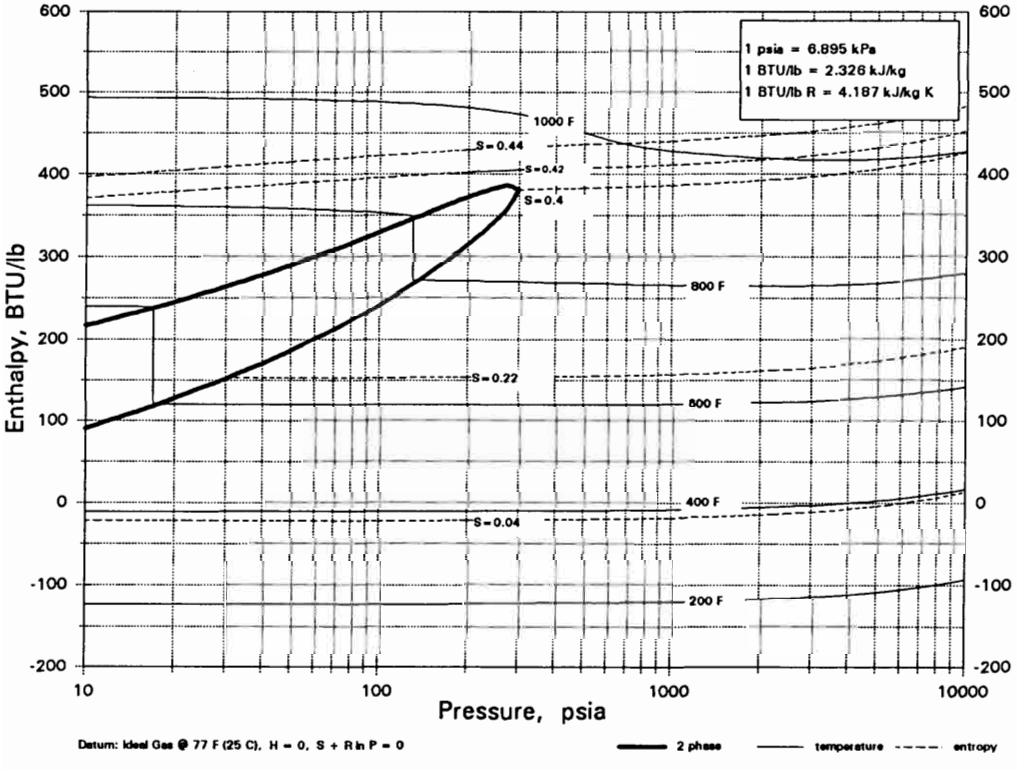
C15H24O 2-6-DI-tert-BUTYL-p-CRESOL



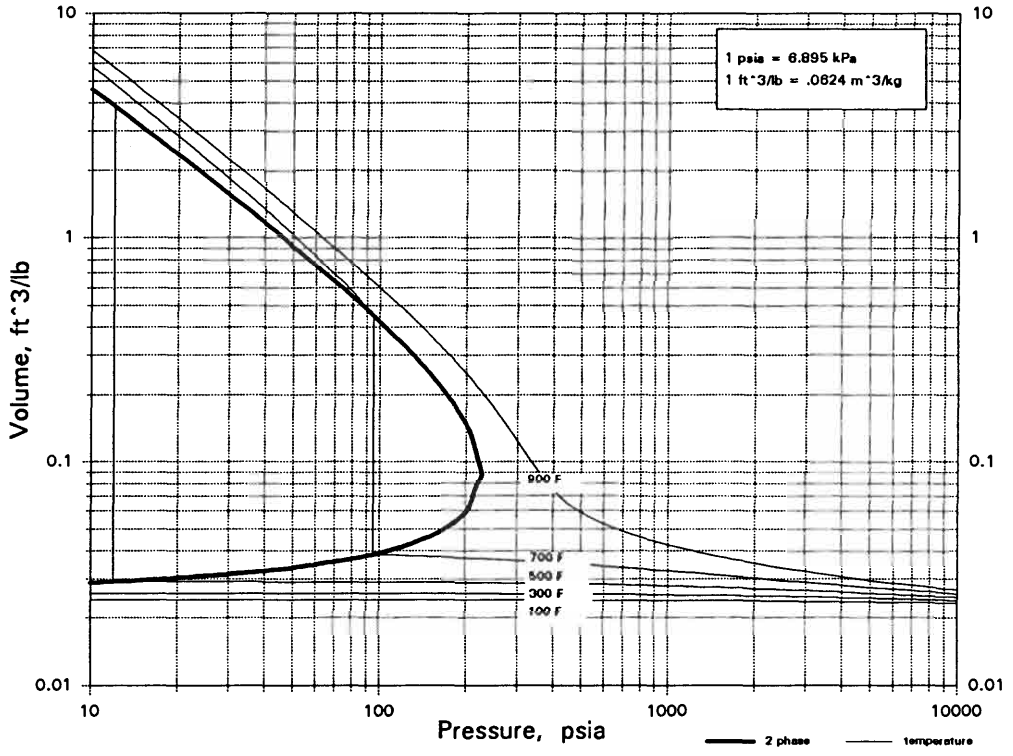


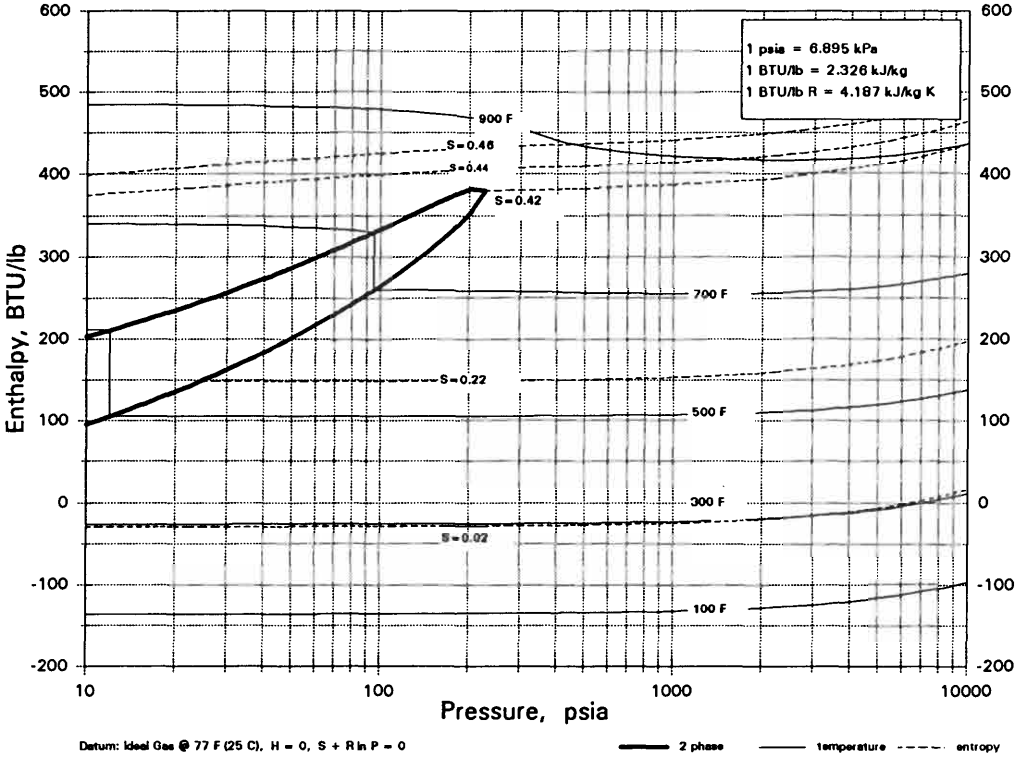
C15H24O NONYLPHENOL



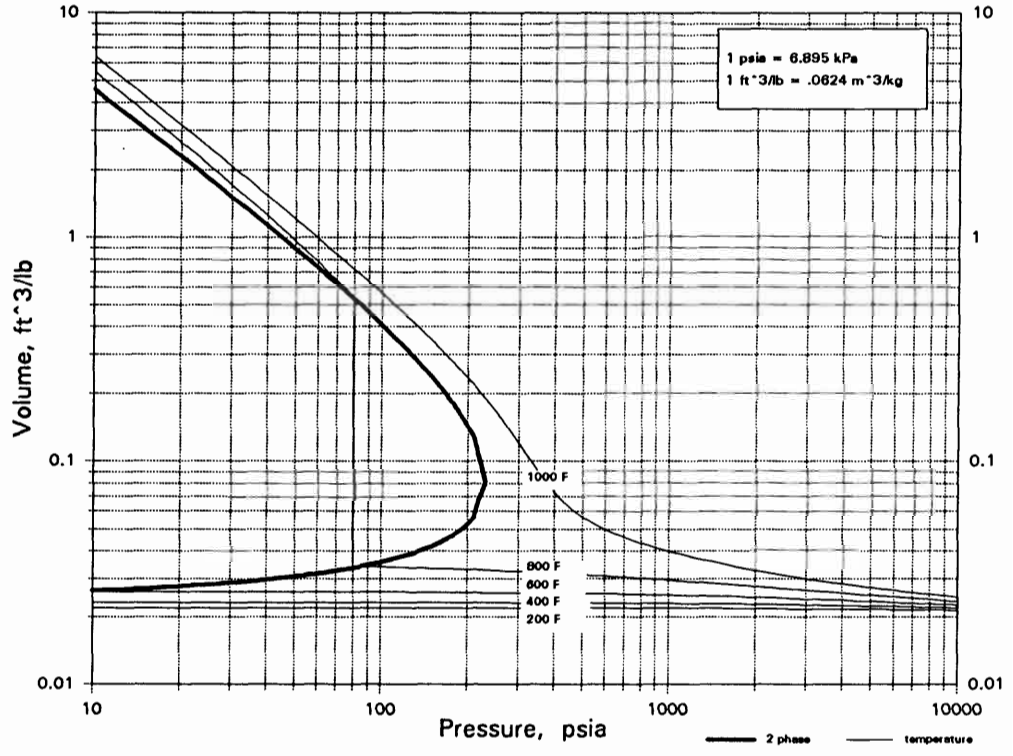


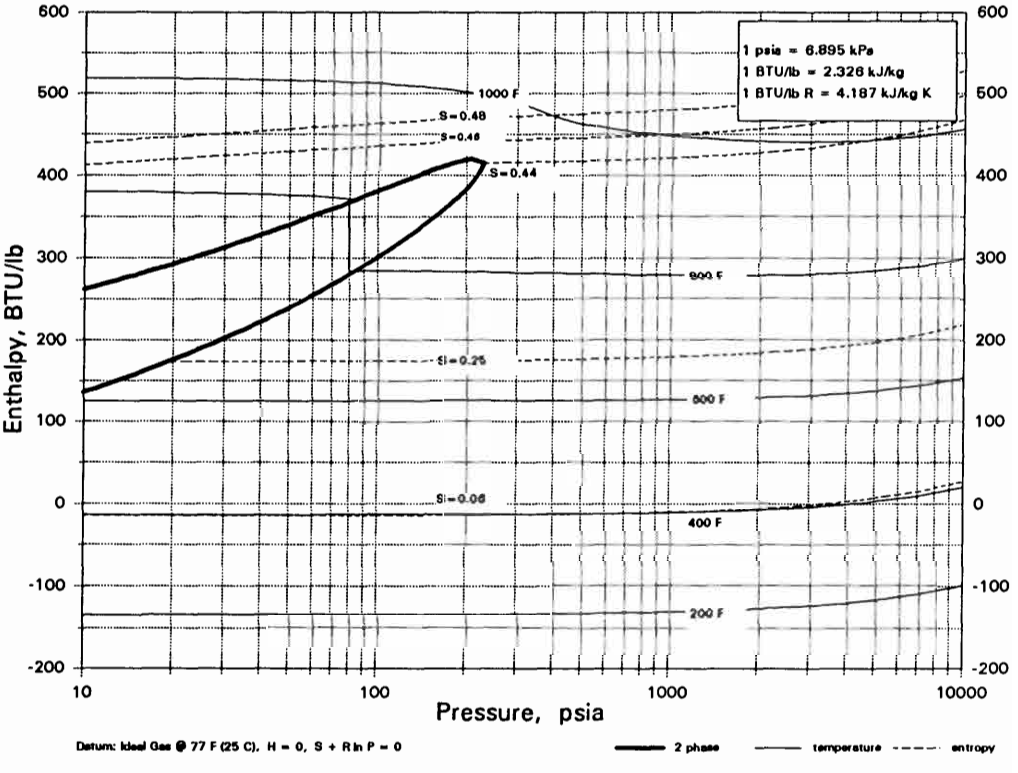
C15H30 1-PENTADECENE



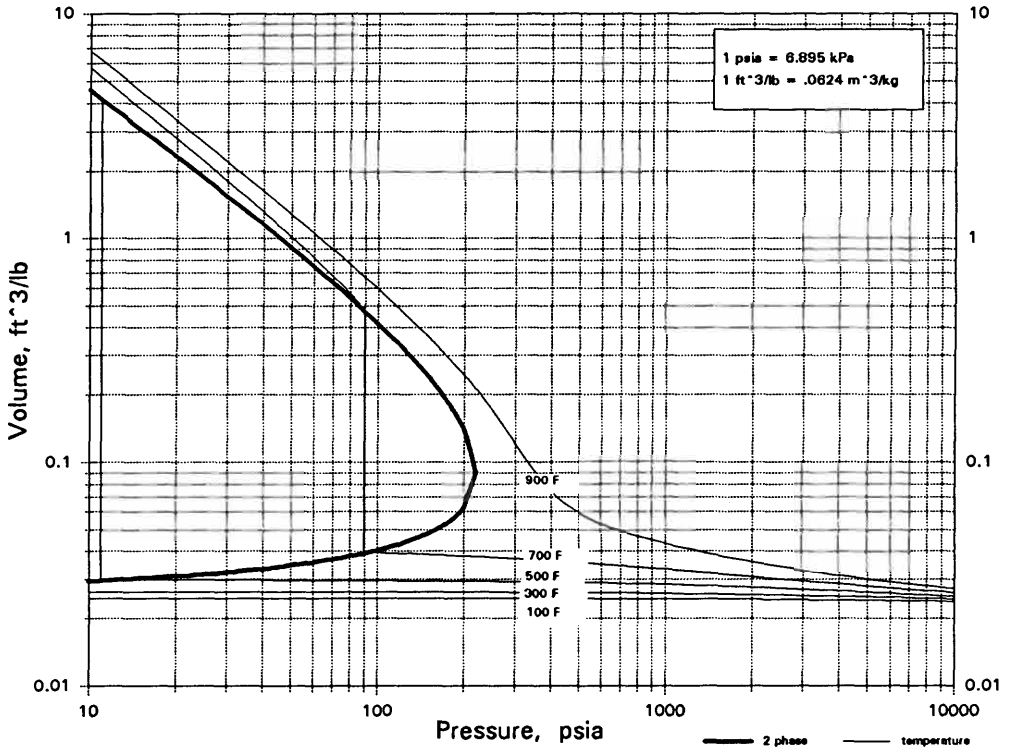


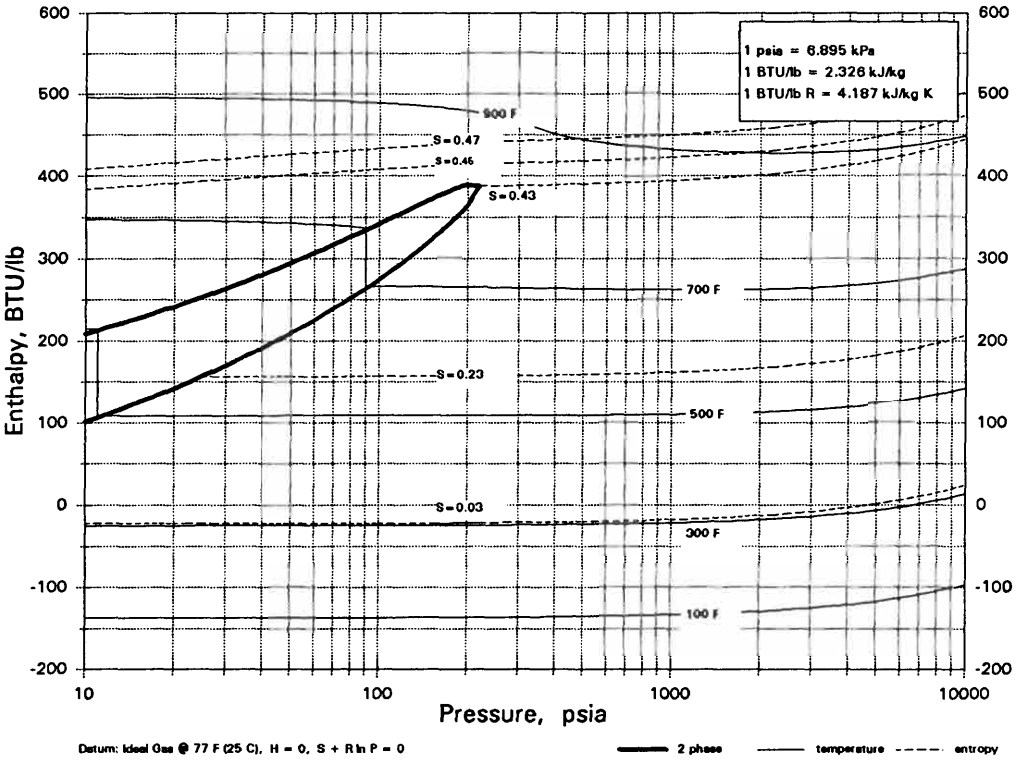
C15H30O2 PENTADECANOIC ACID



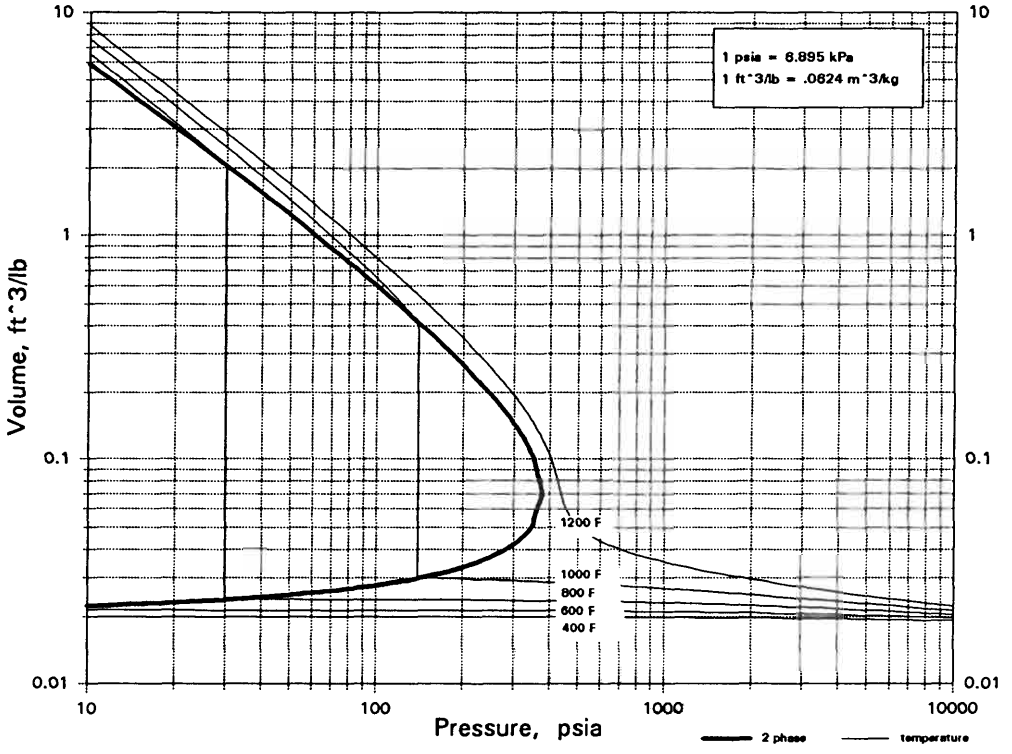


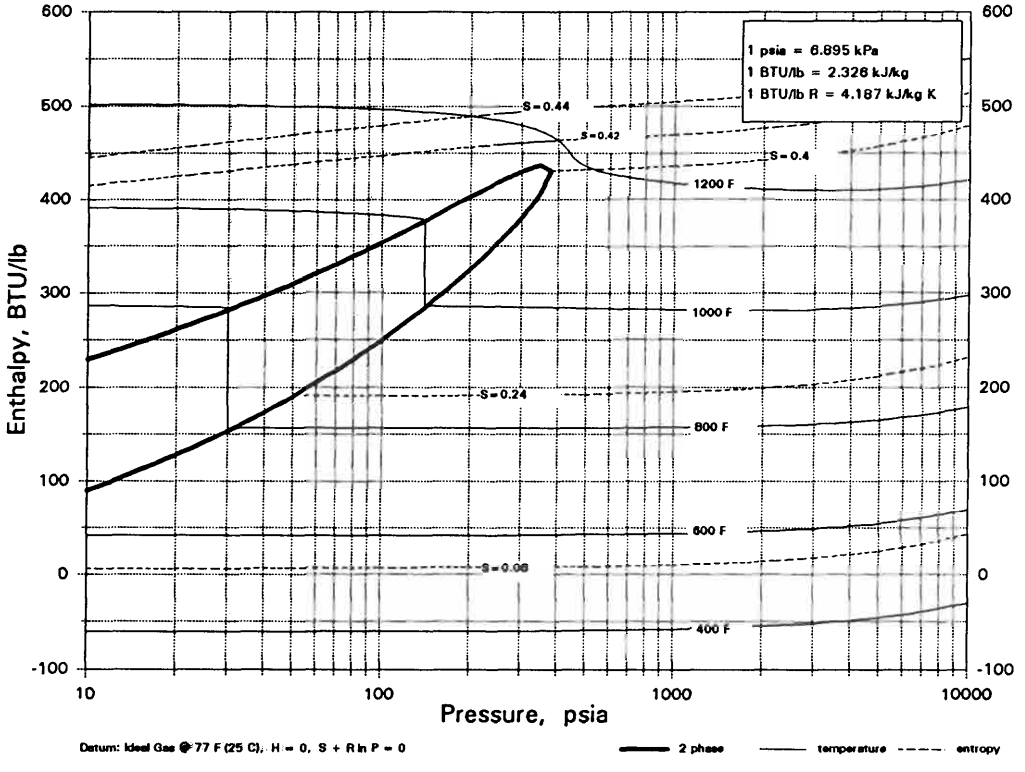
C15H32 n-PENTADECANE



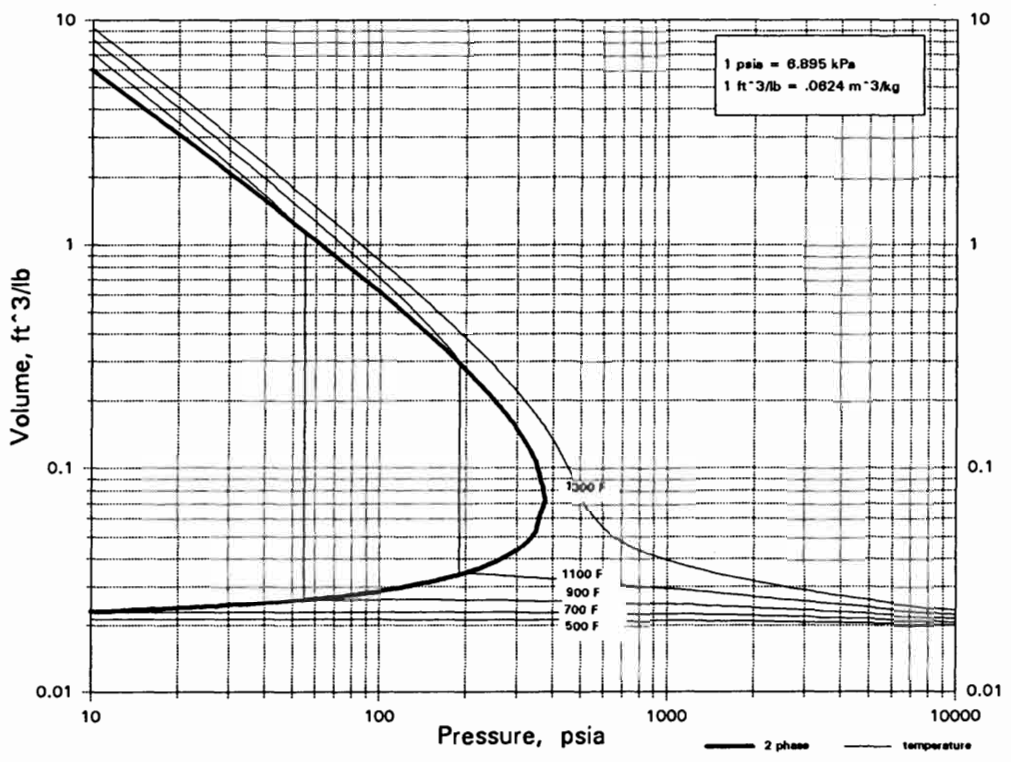


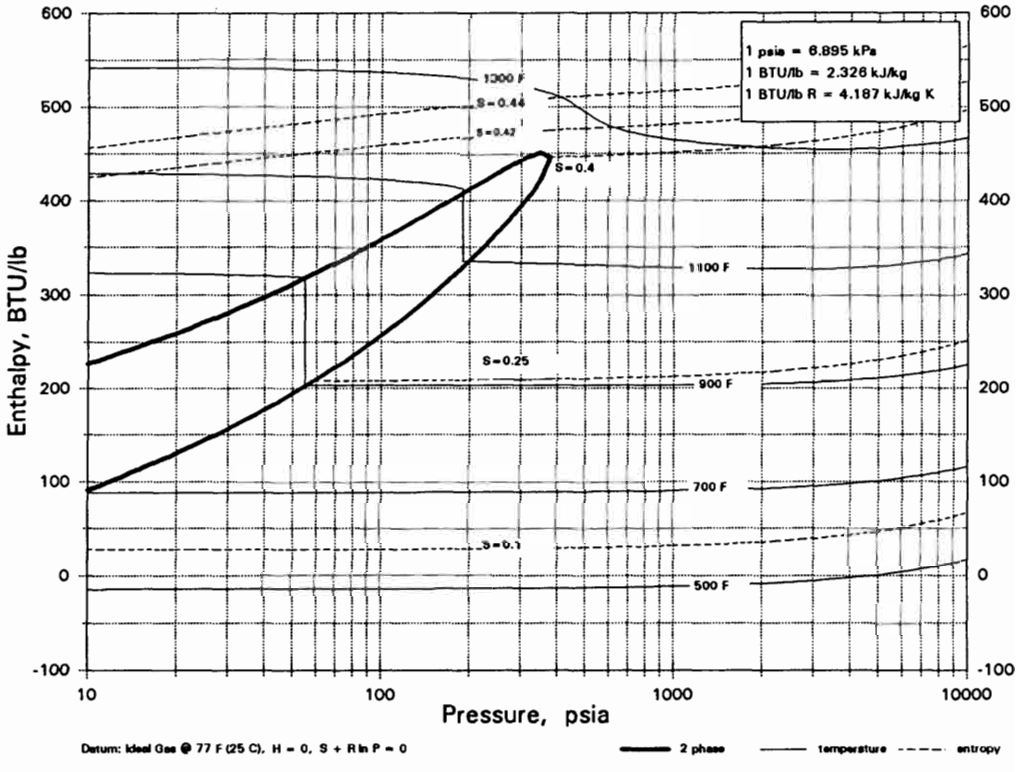
C16H10 FLUORANTHENE



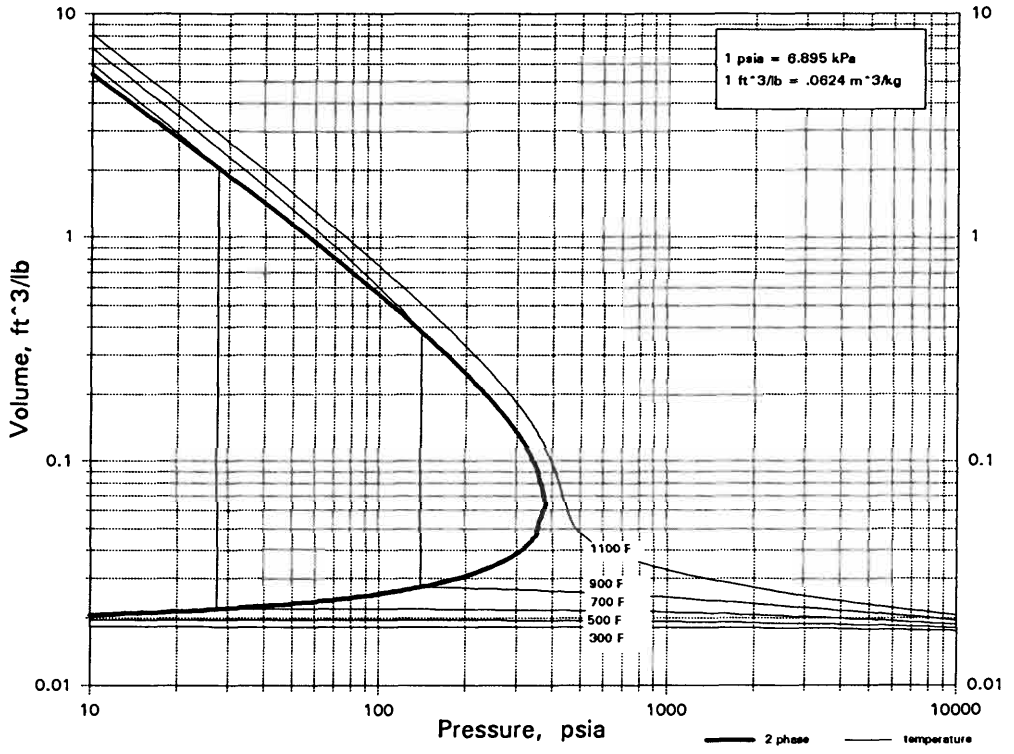


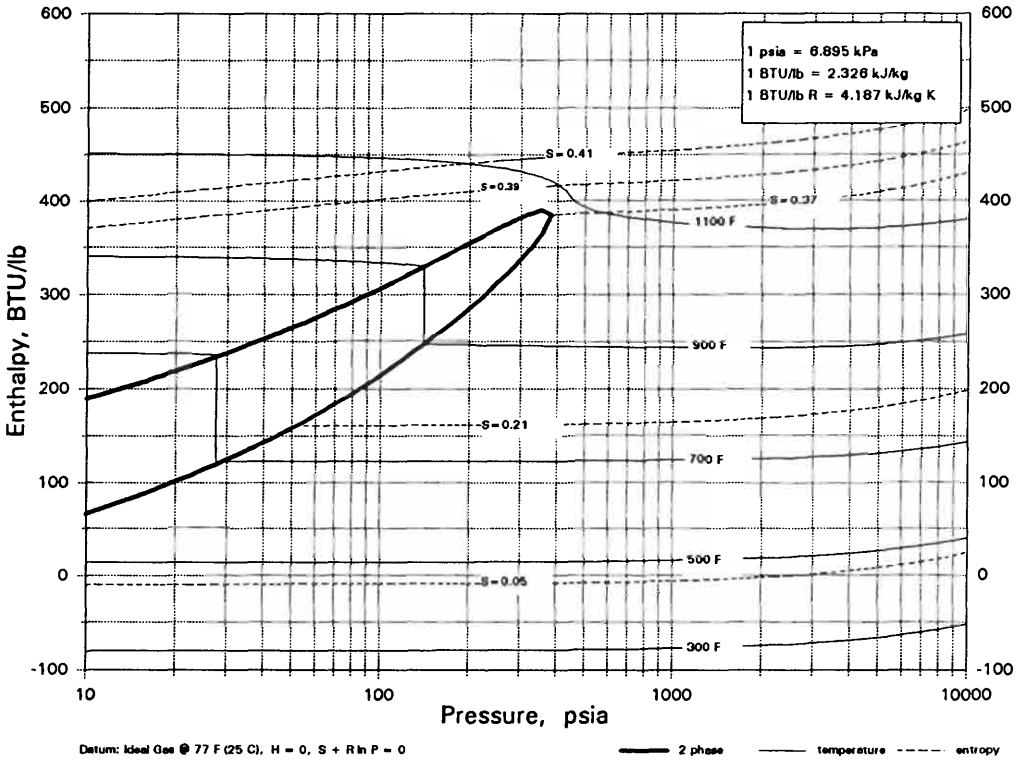
C16H10 PYRENE



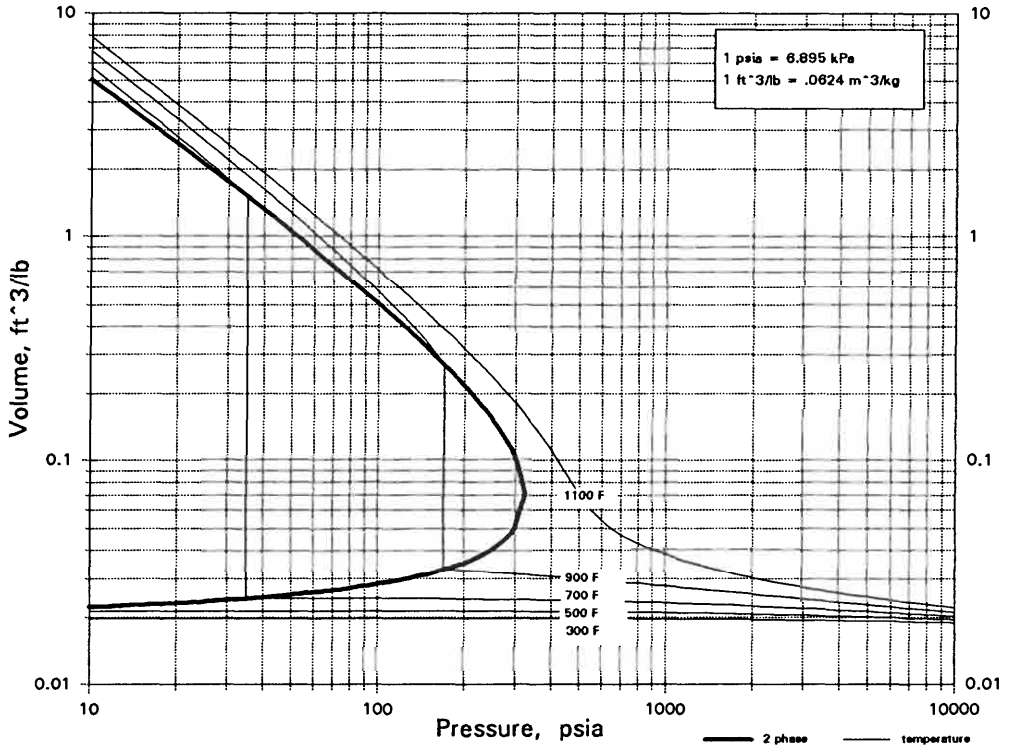


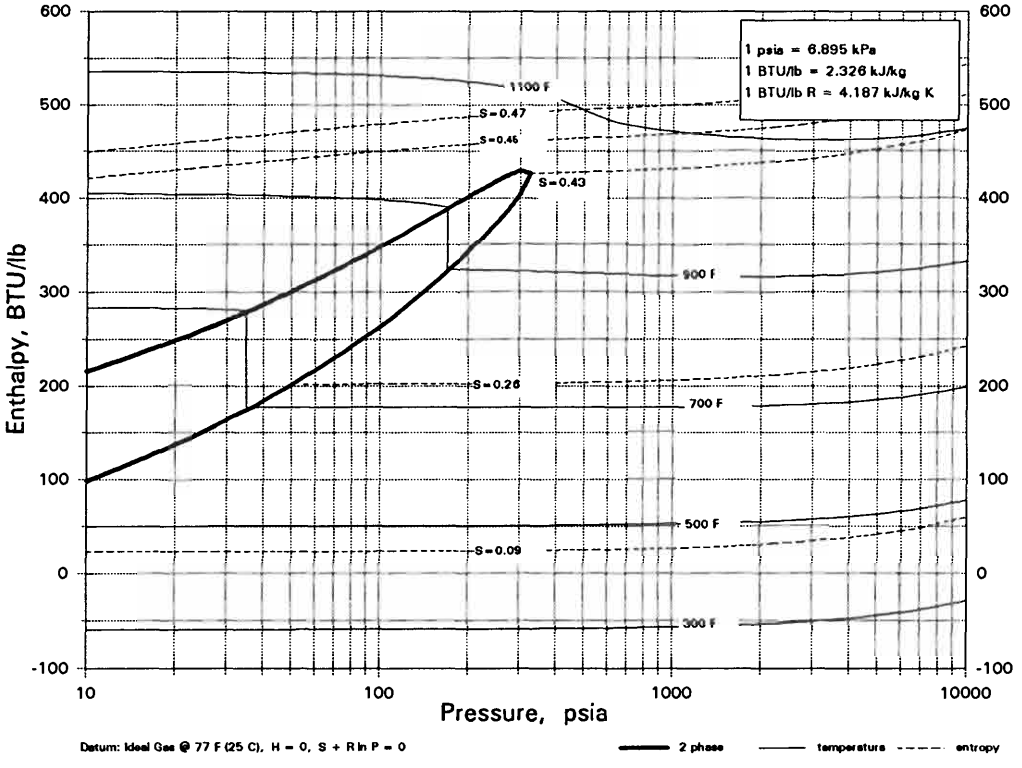
C16H12 1-PHENYLNAPHTHALENE



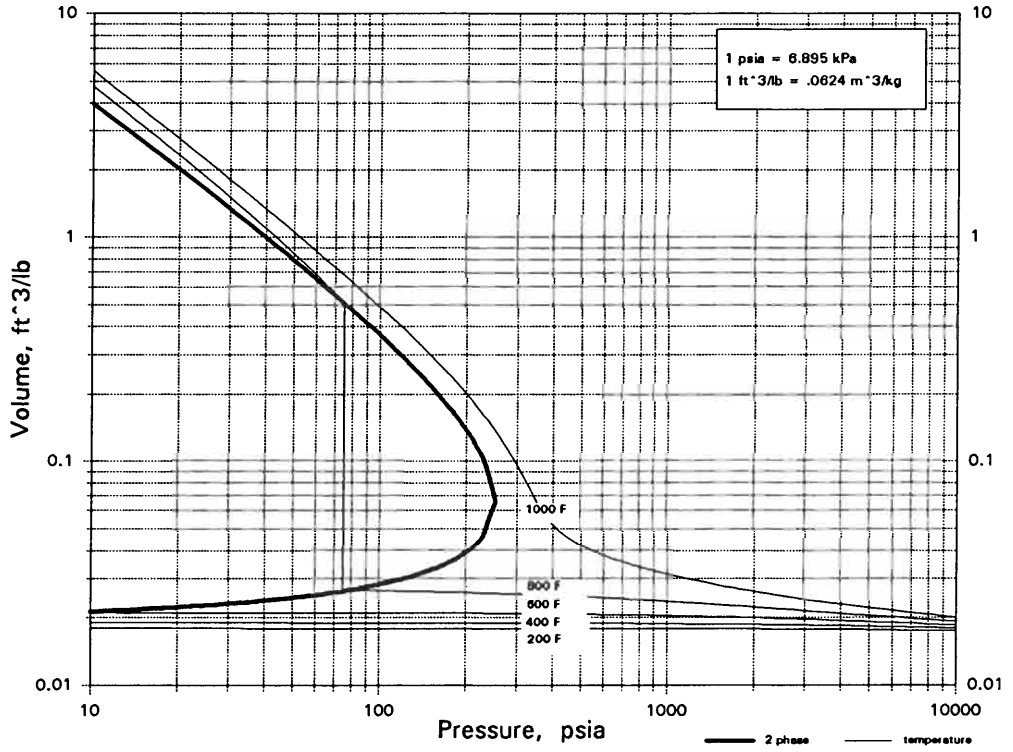


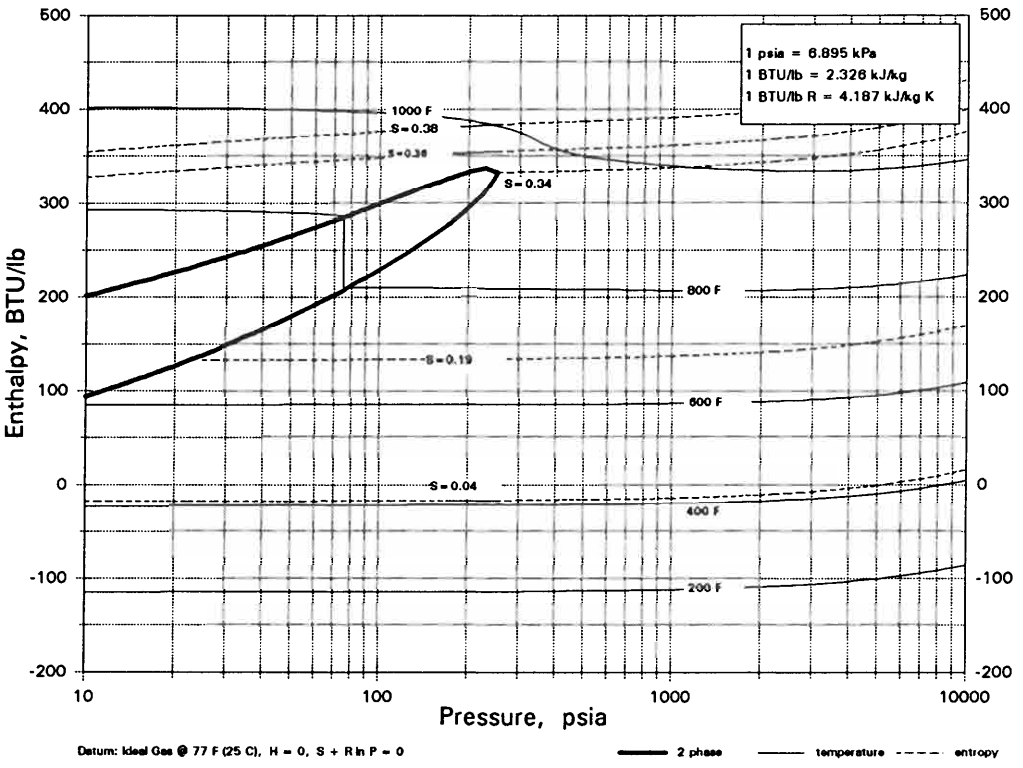
C16H20 1-n-HEXYLNAPHTHALENE



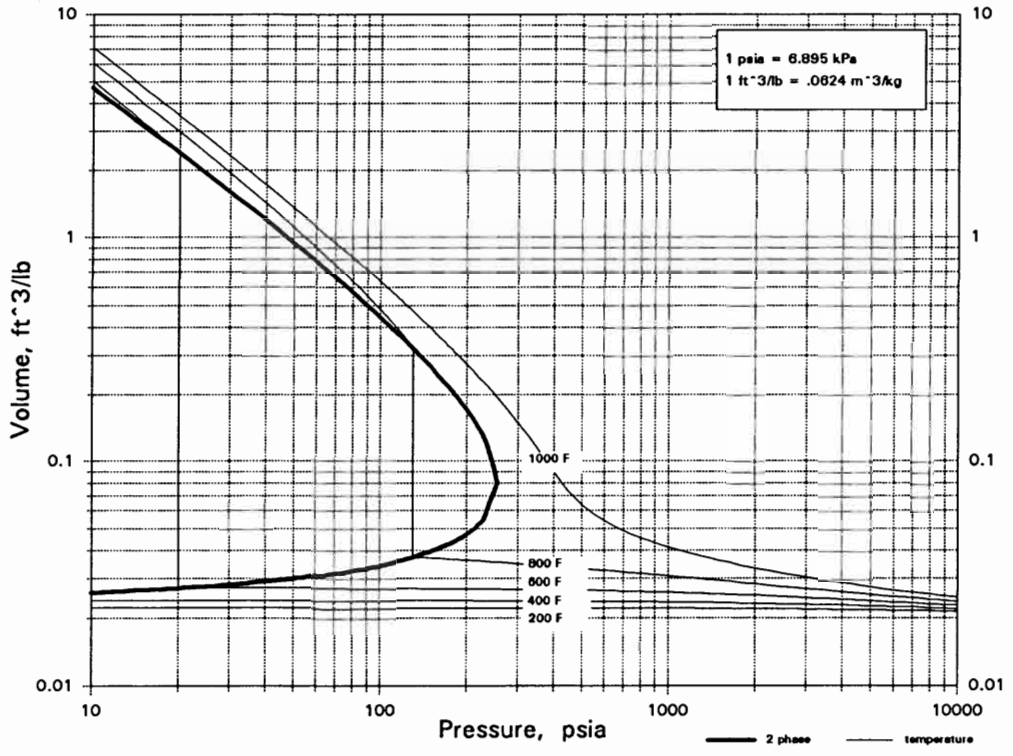


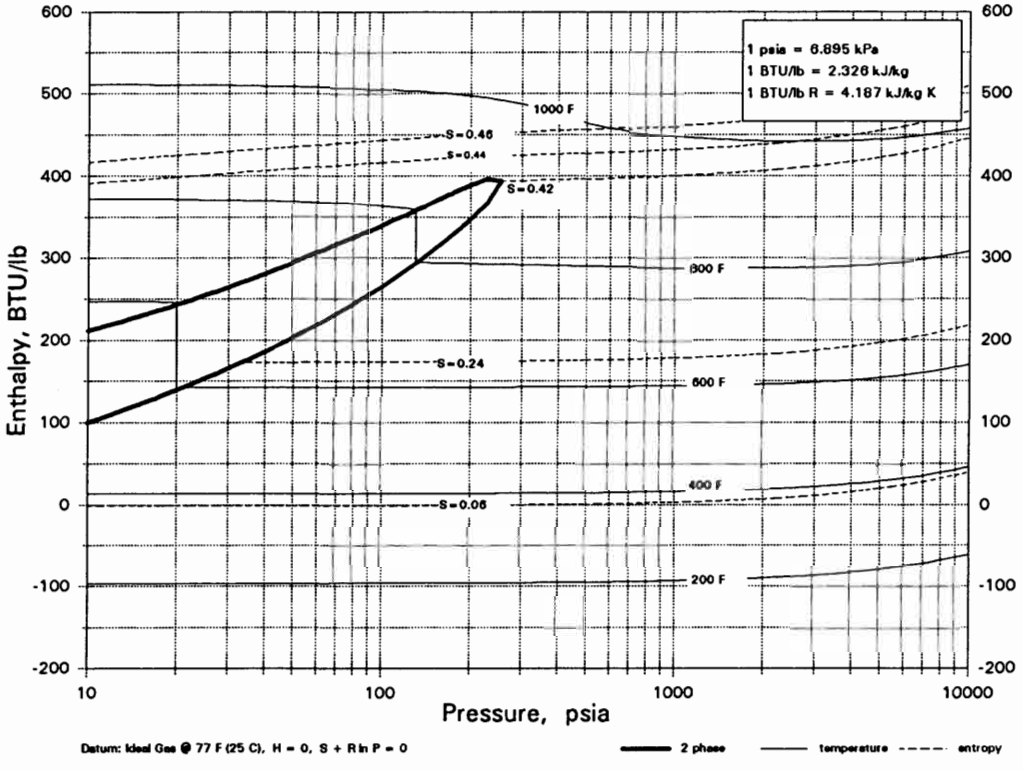
C16H22O4 DIBUTYL PHTHALATE



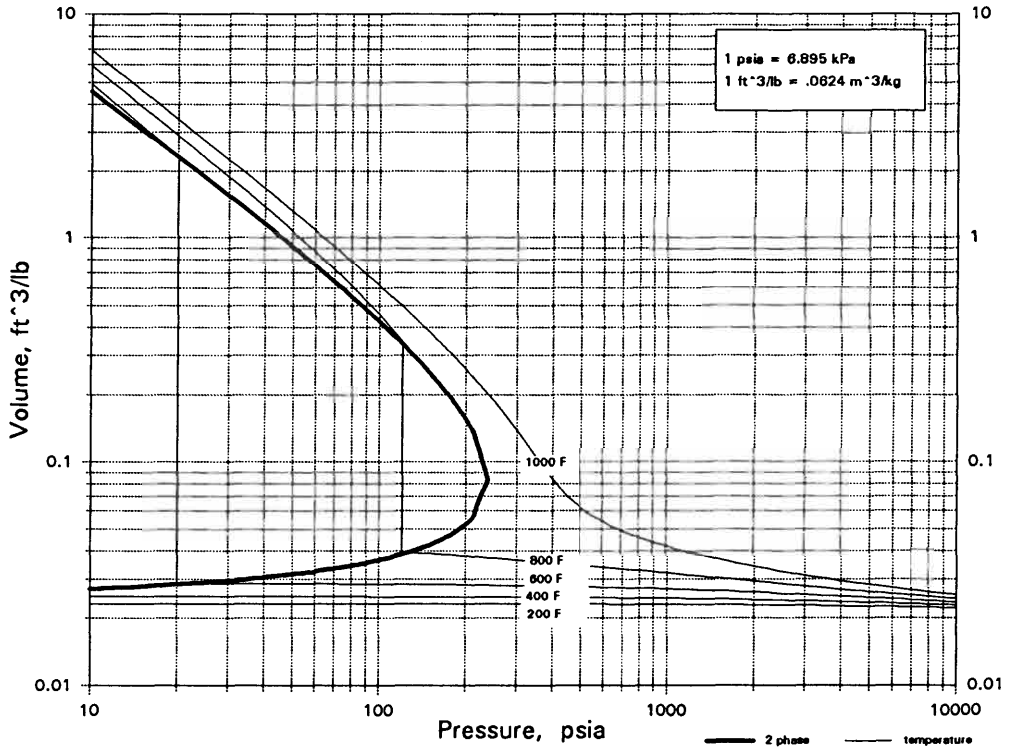


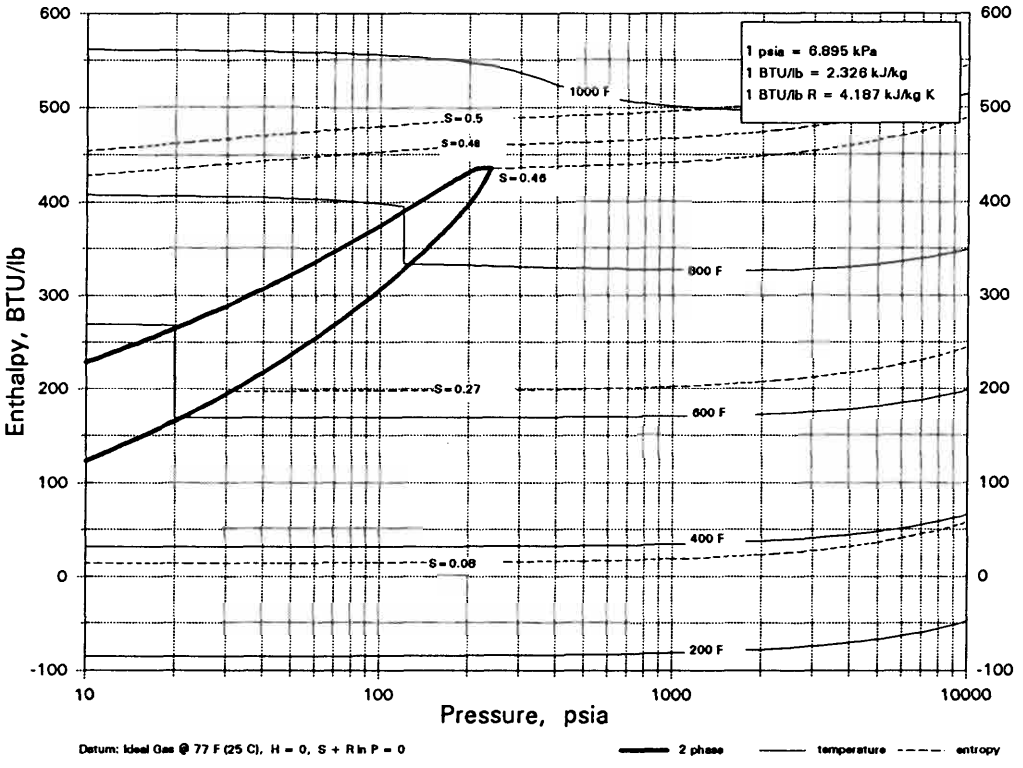
C16H26 n-DECYLBENZENE



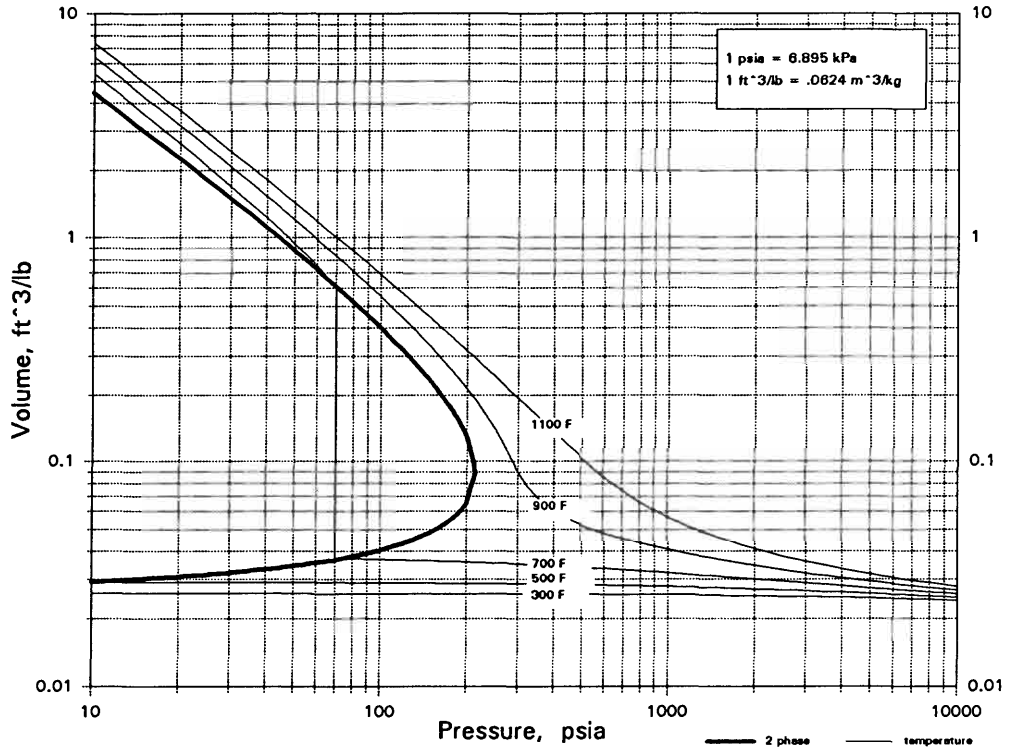


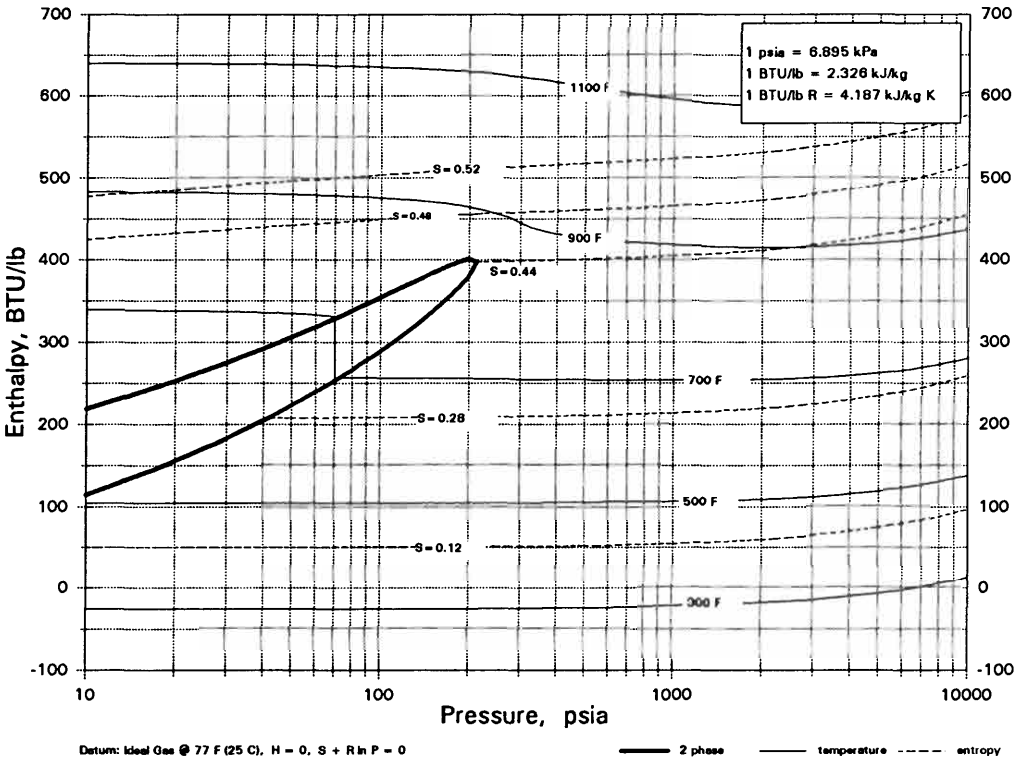
C16H32 n-DECYLCYCLOHEXANE



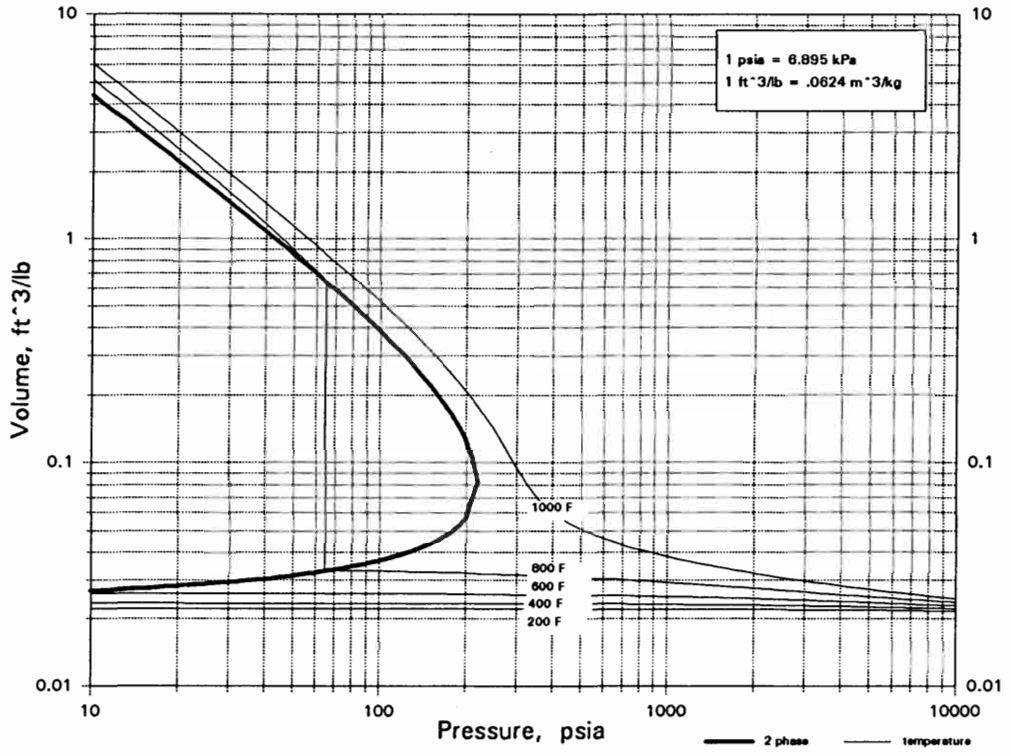


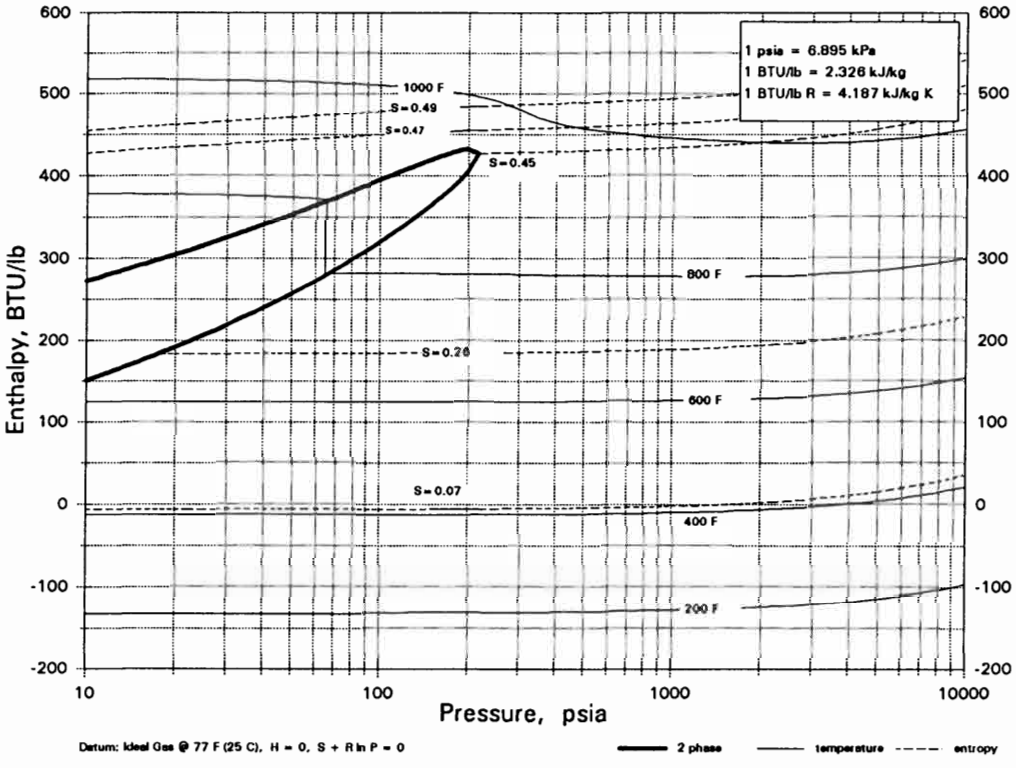
C16H32 1-HEXADECENE



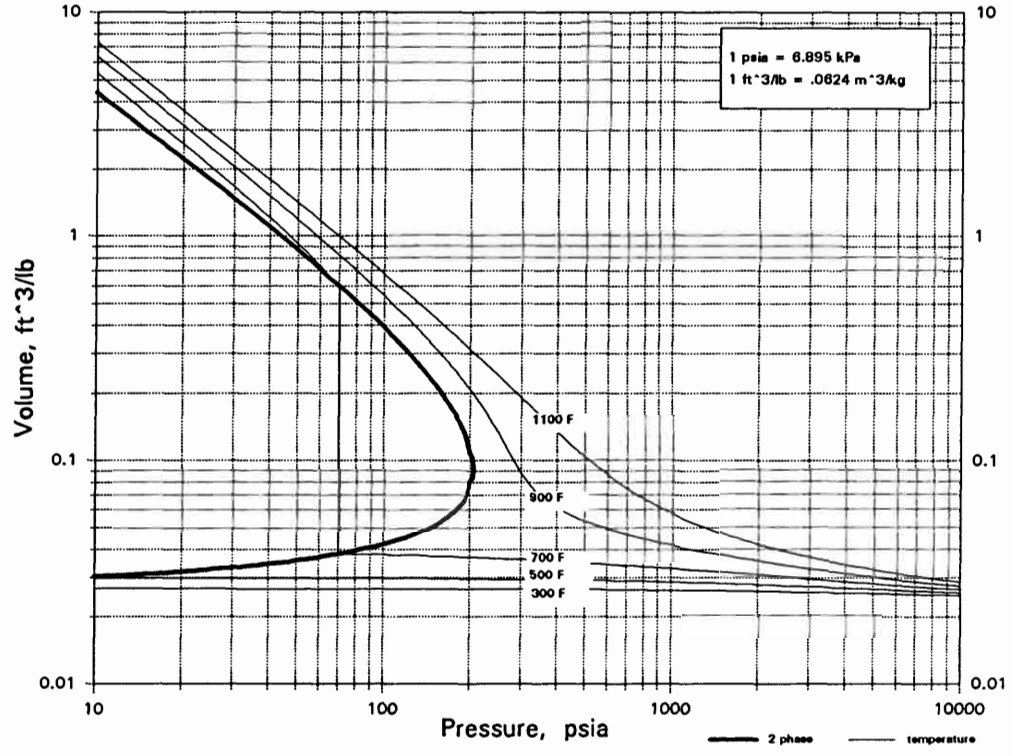


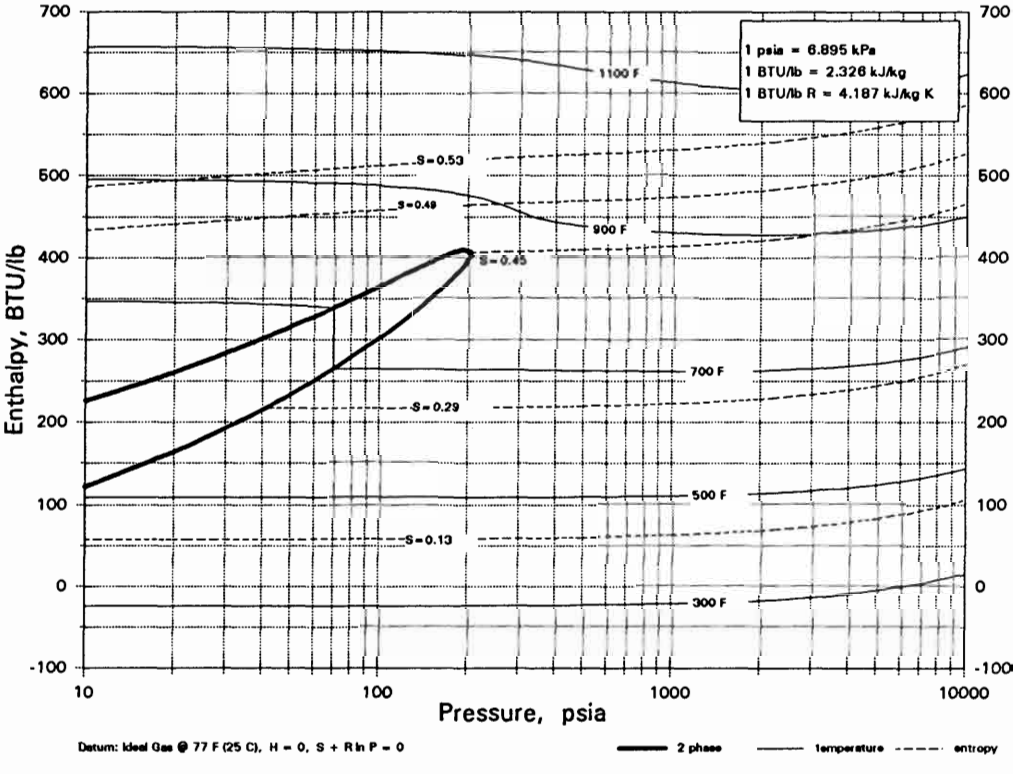
C16H32O2 n-HEXADECANOIC ACID



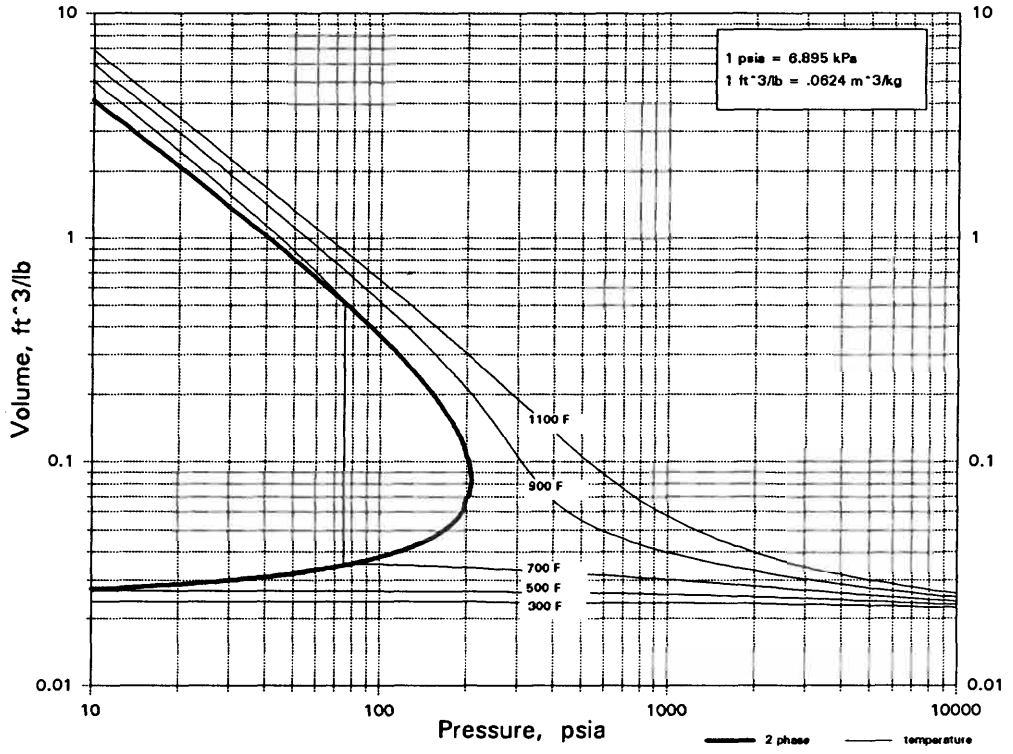


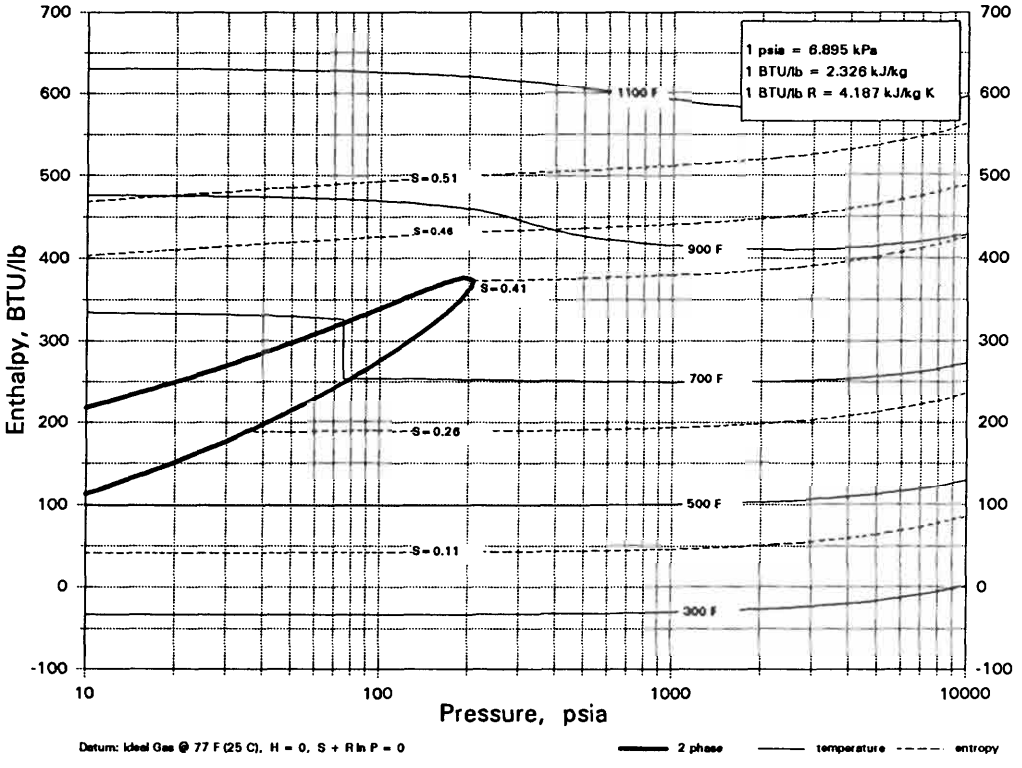
C16H34 n-HEXADECANE



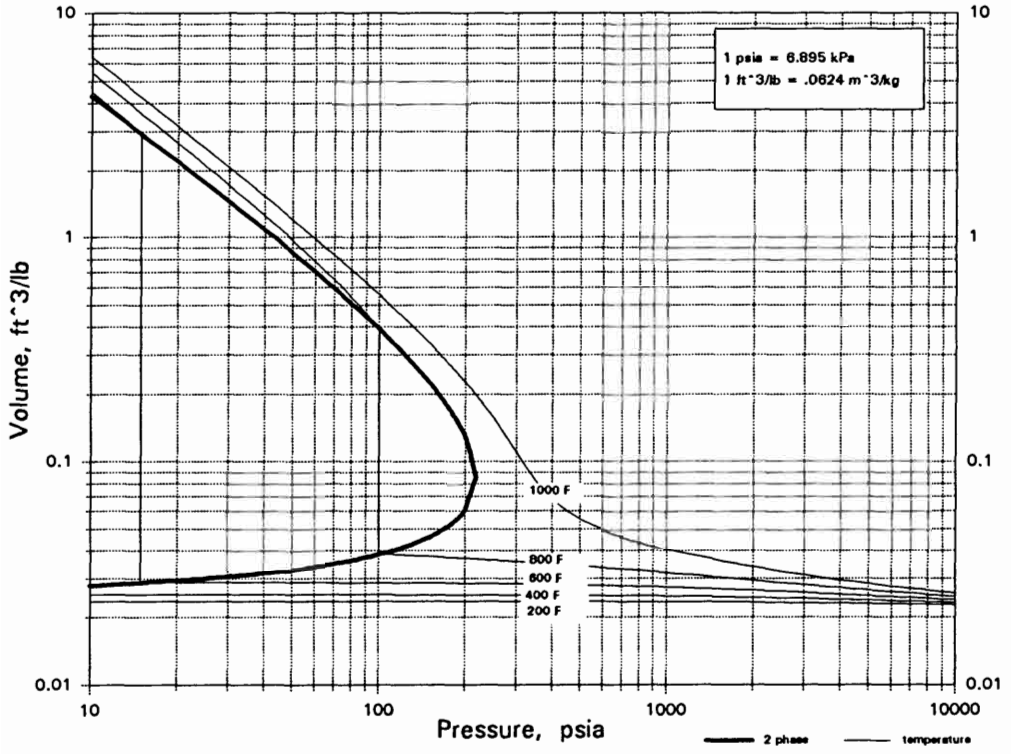


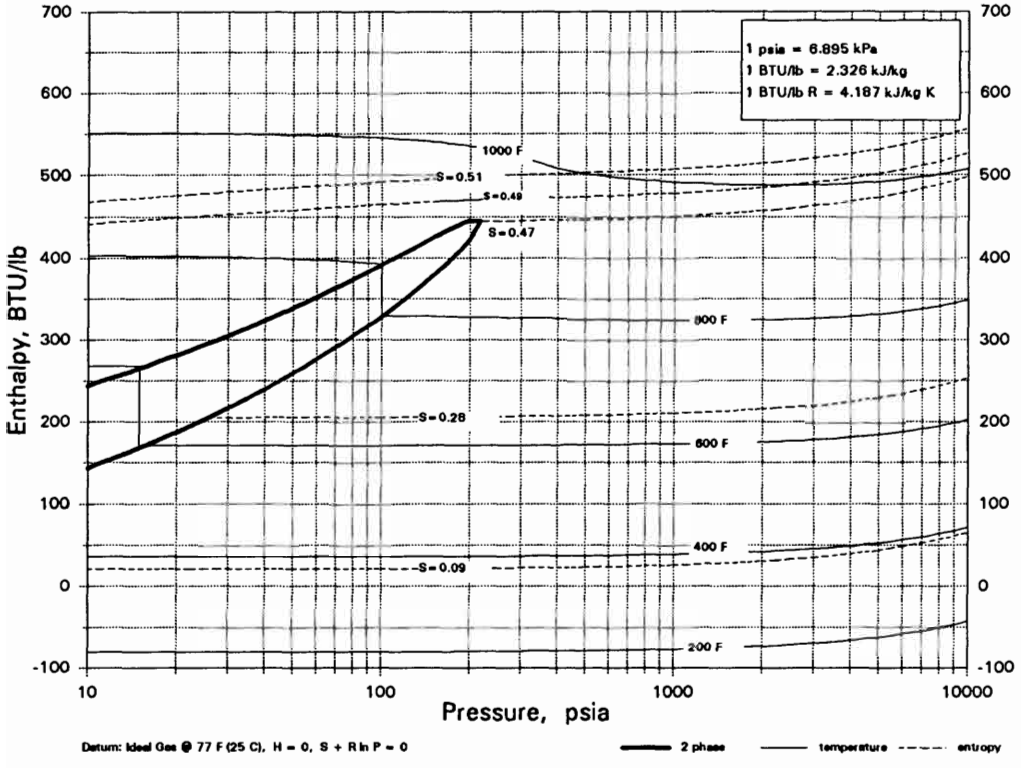
C16H34O DI-n-OCTYL ETHER



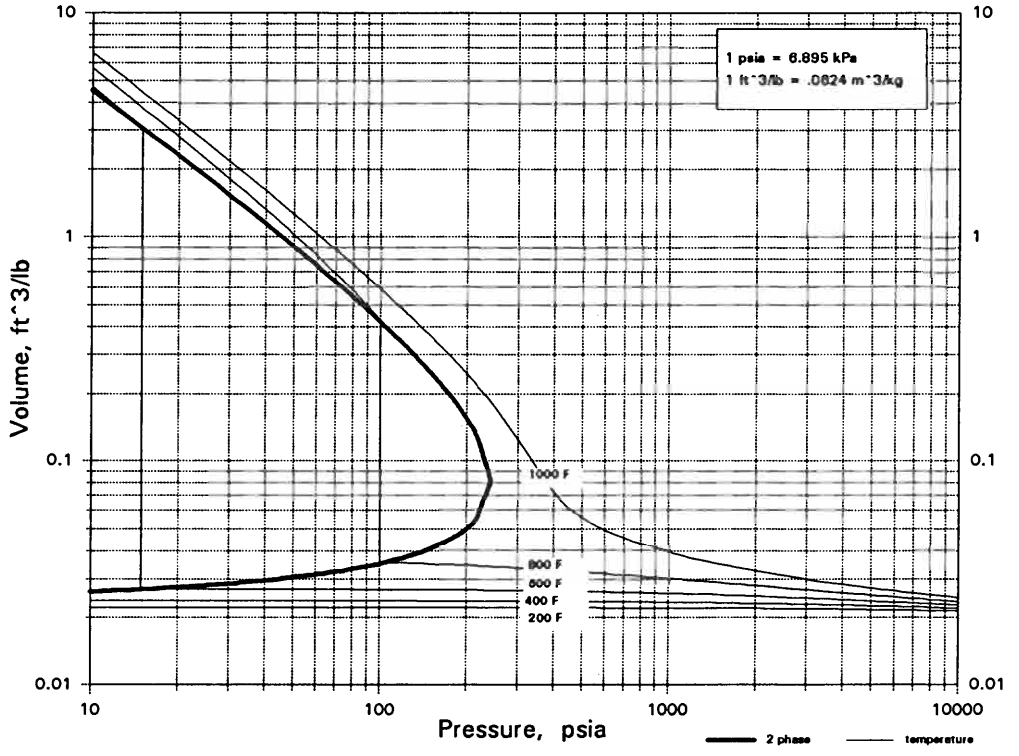


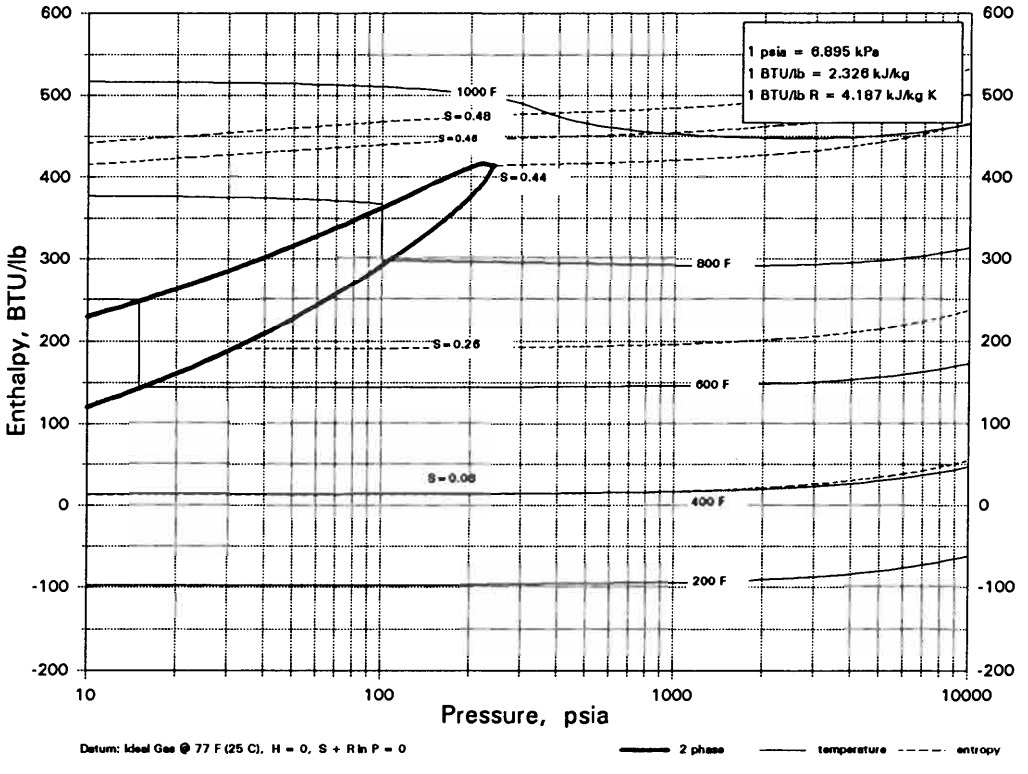
C16H34O 1-HEXADECANOL



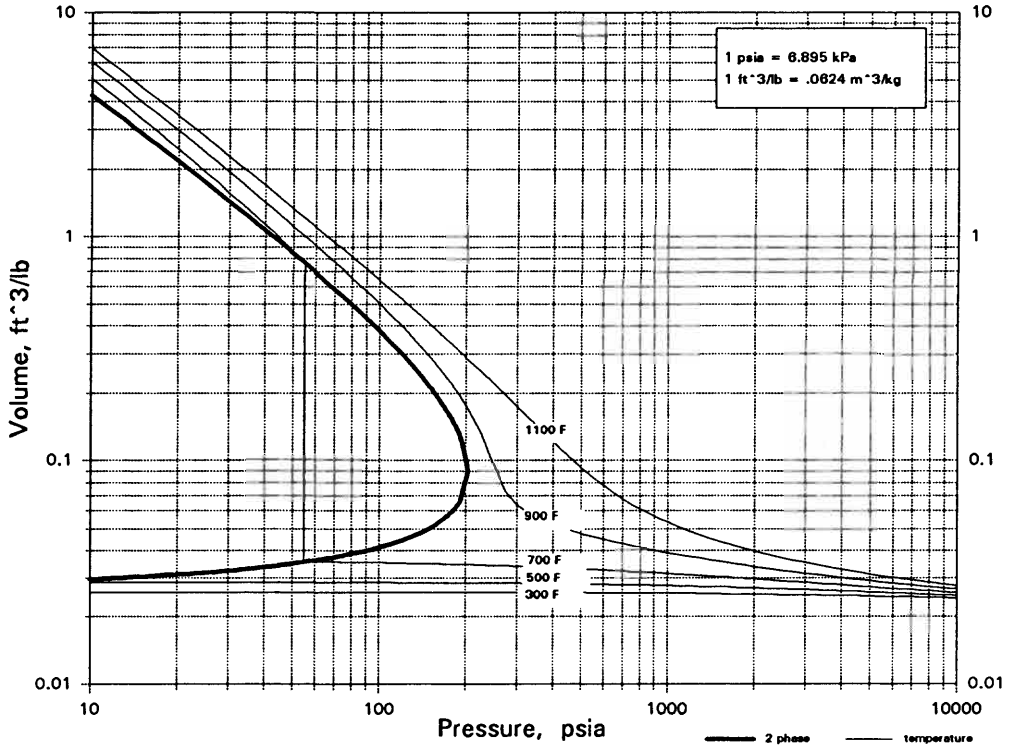


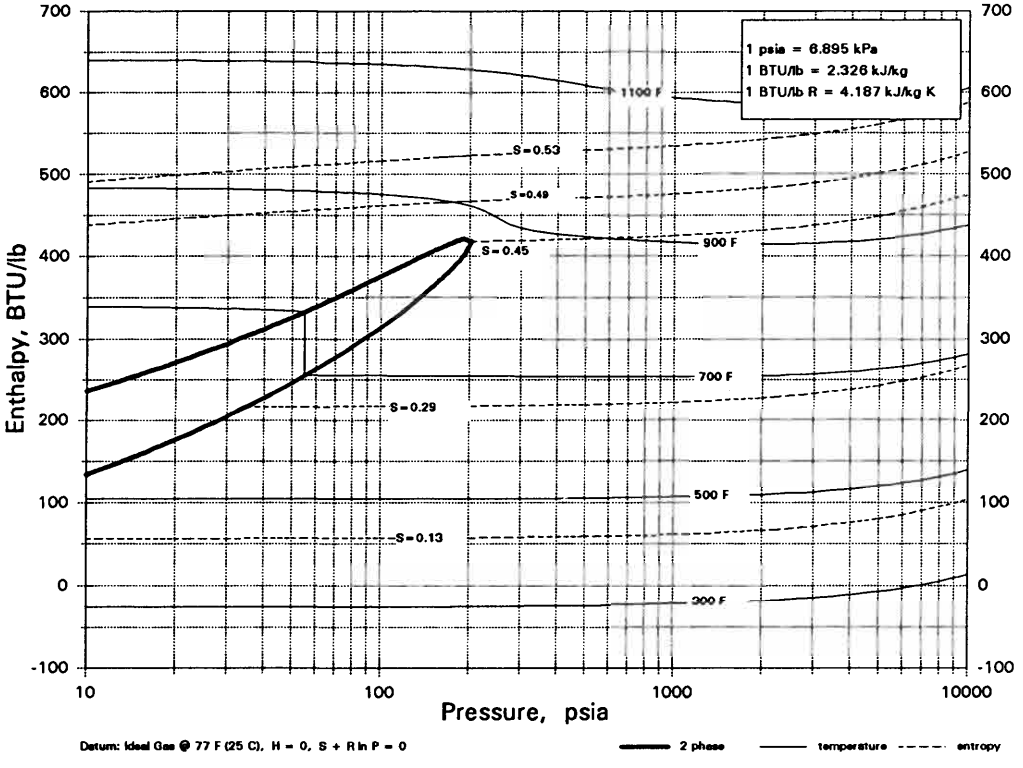
C17H28 n-UNDECYLBENZENE



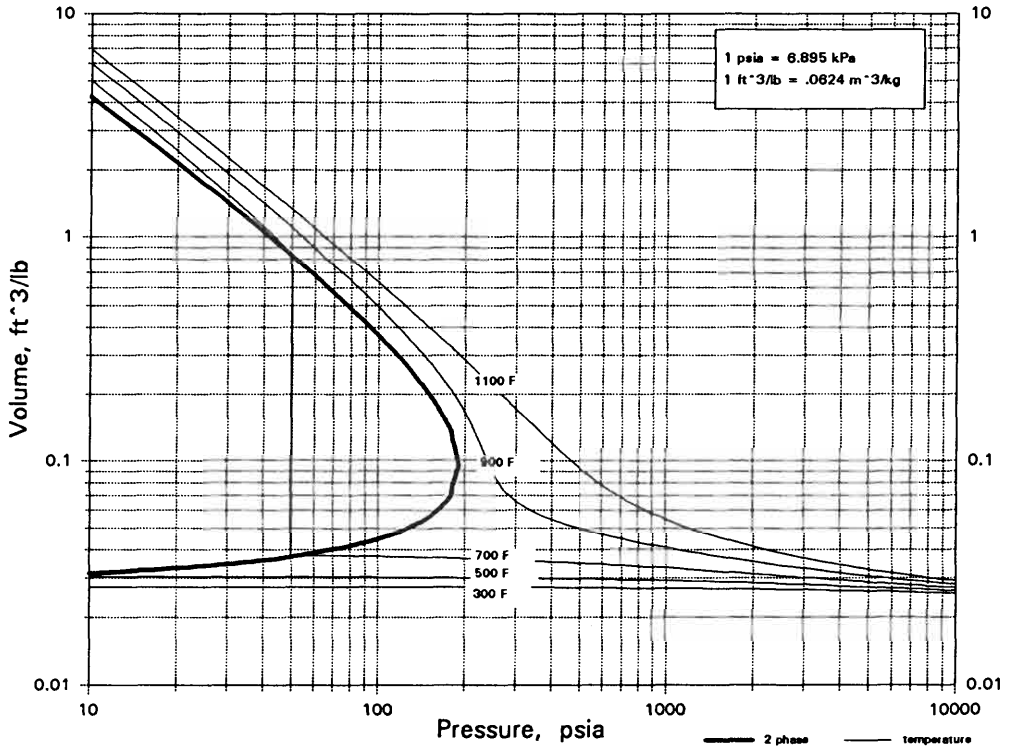


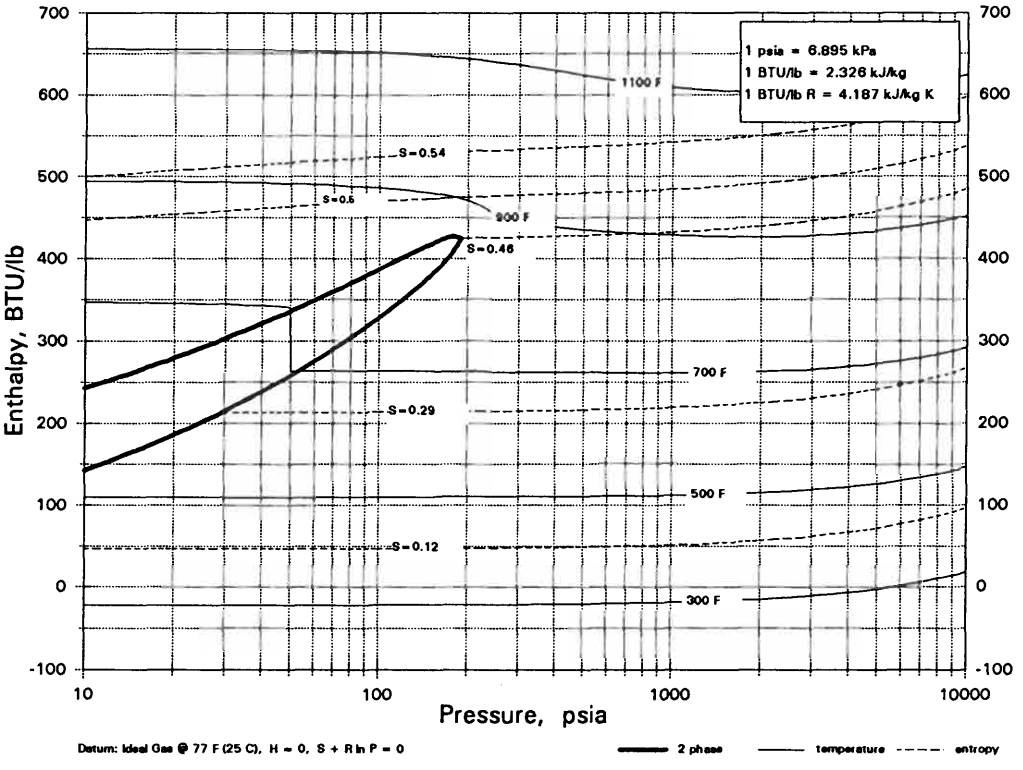
C17H34 1-HEPTADECENE



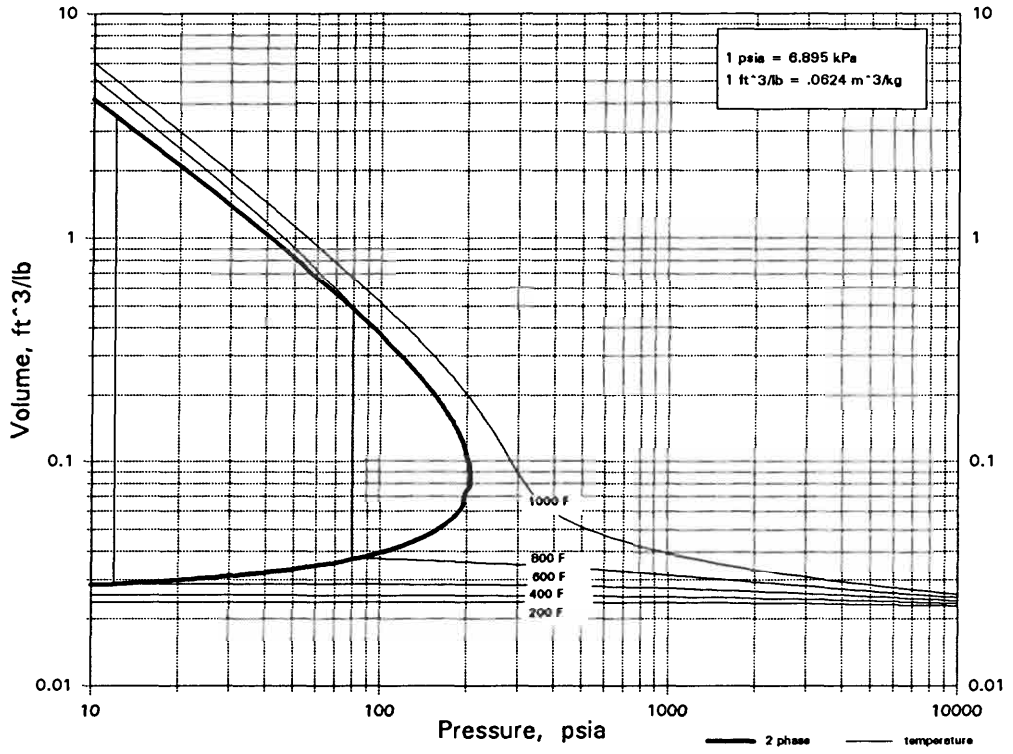


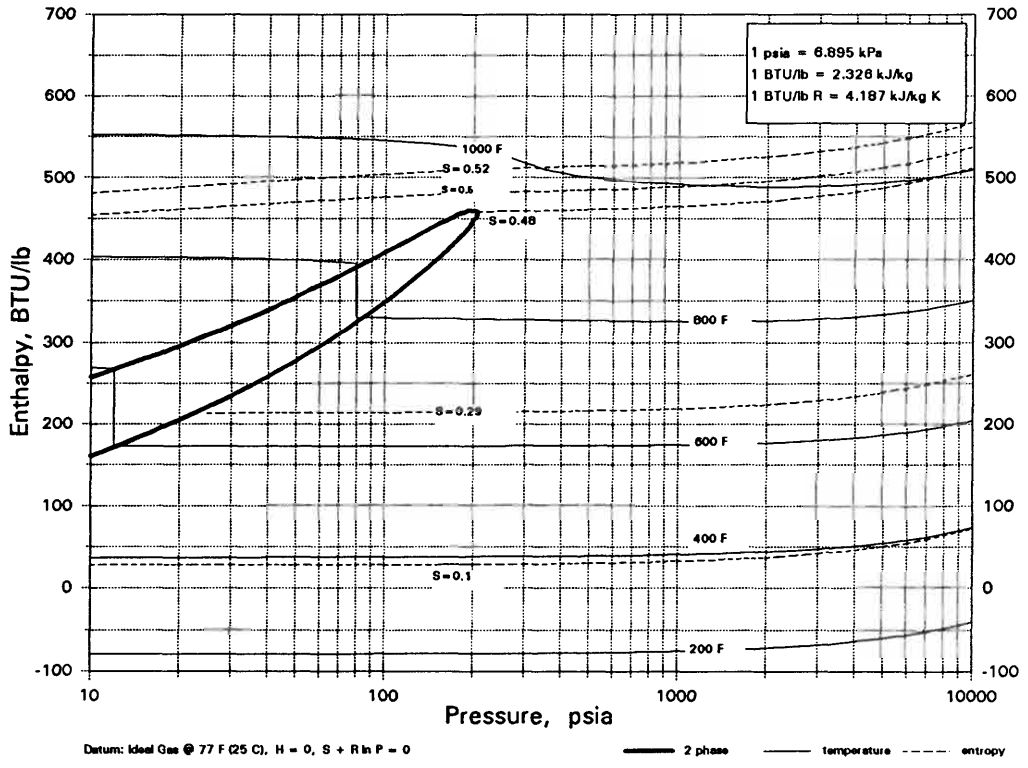
C17H36 n-HEPTADECANE



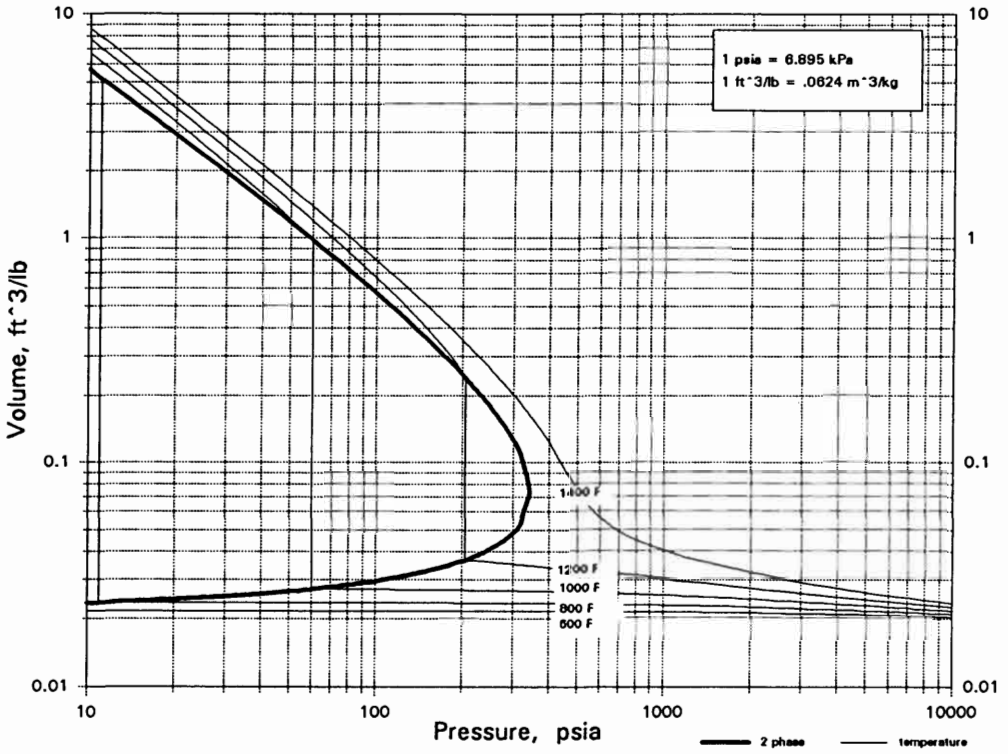


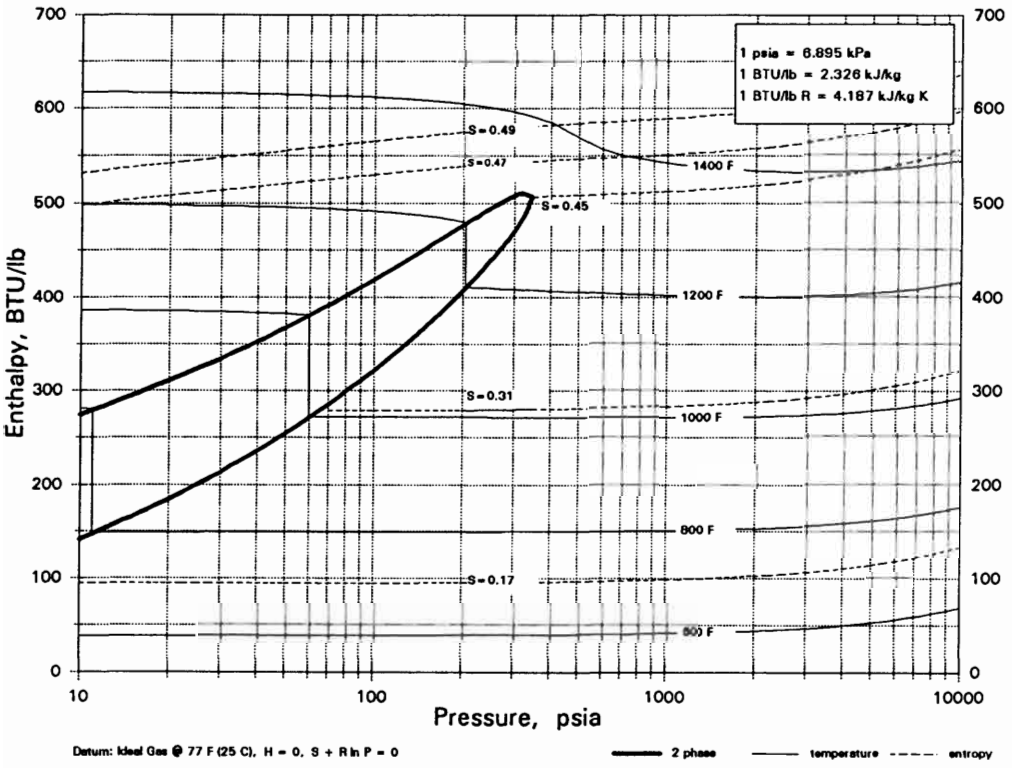
C17H36O 1-HEPTADECANOL



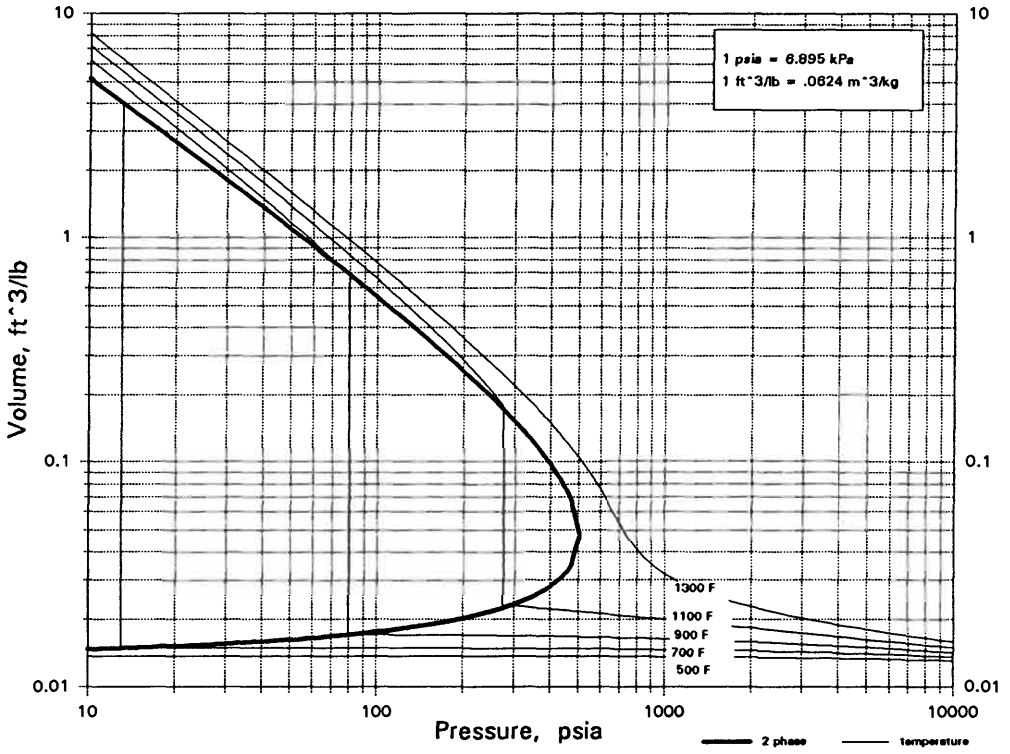


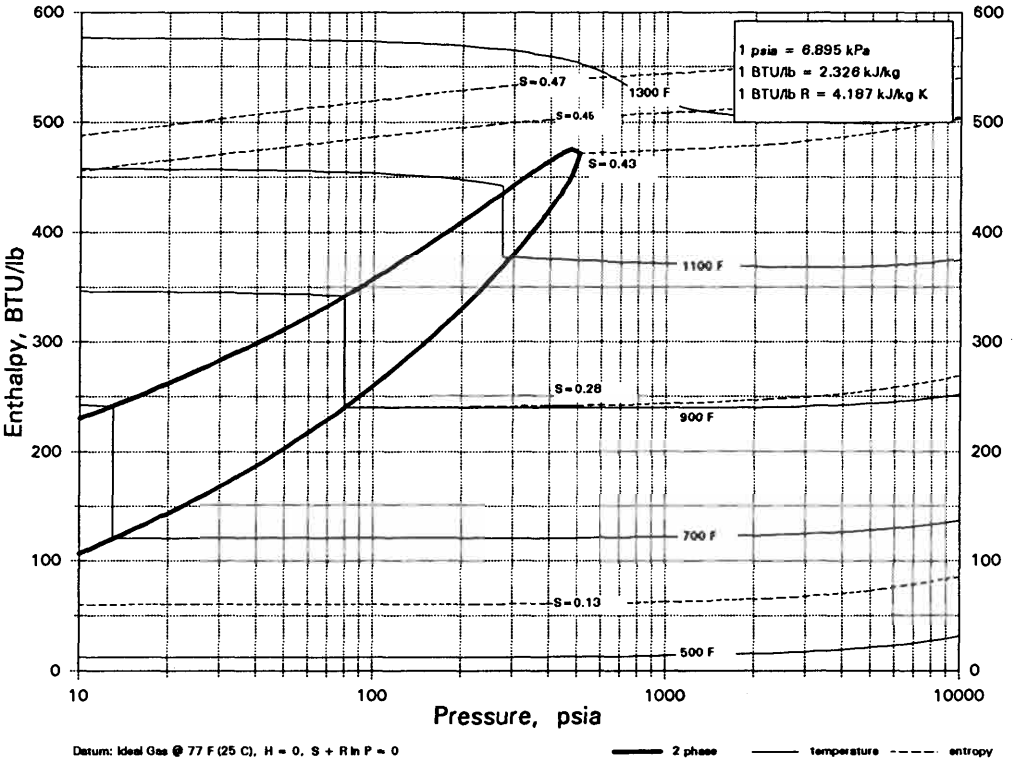
C18H12 CHRYSENE



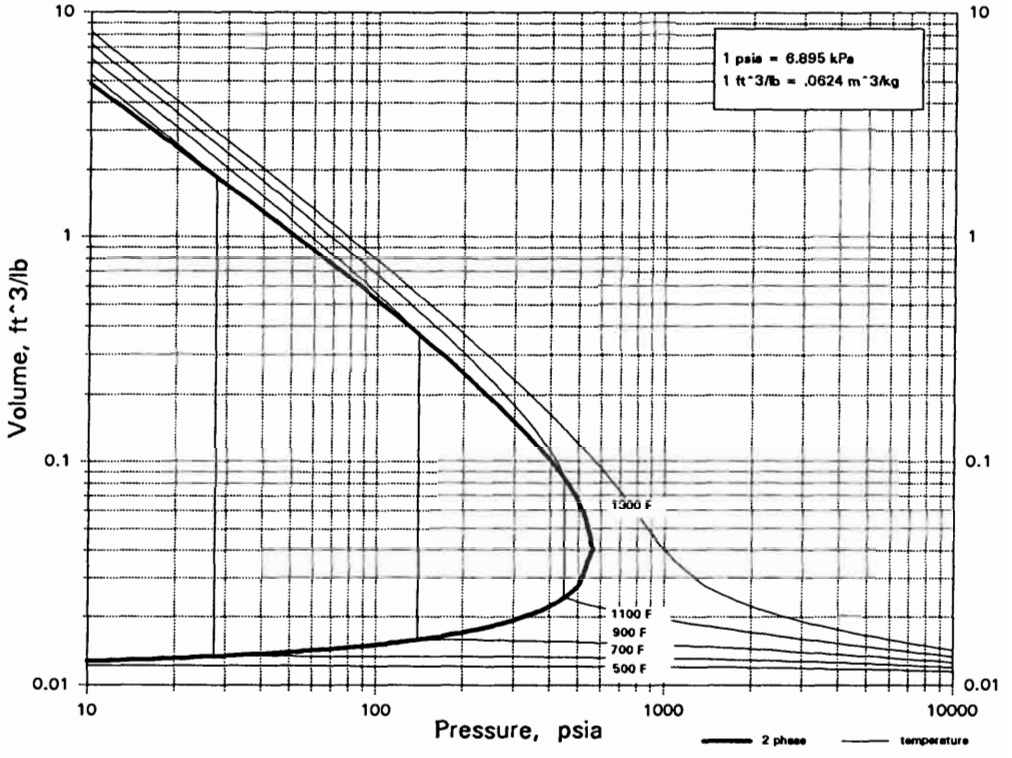


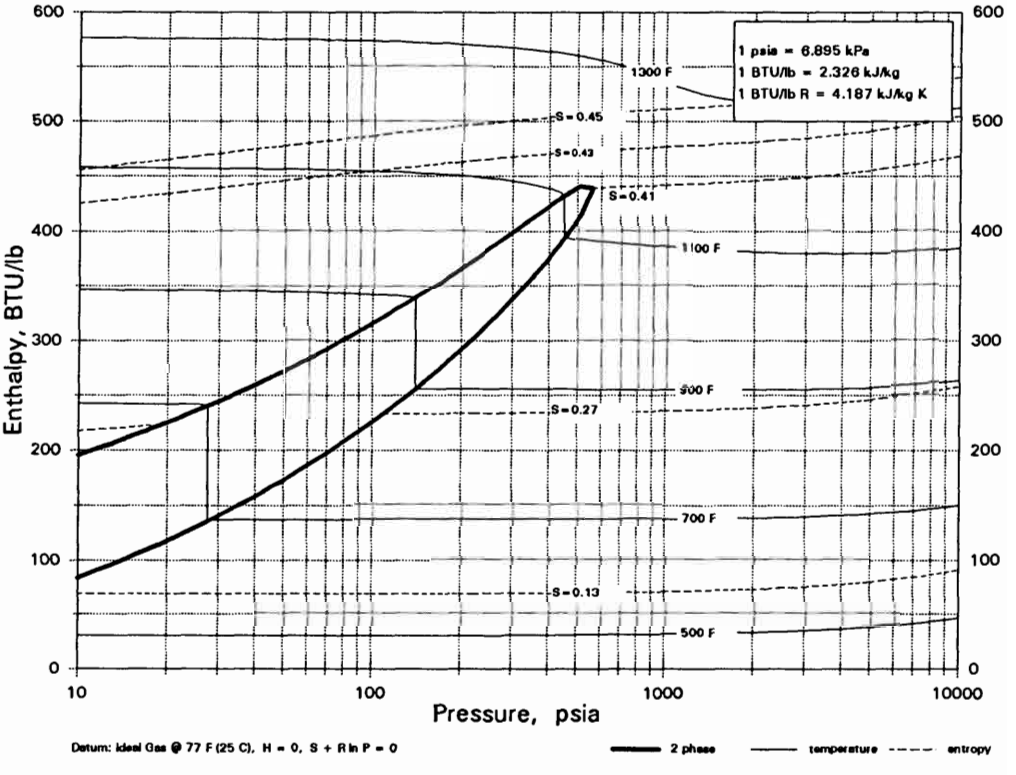
C18H14 m-TERPHENYL



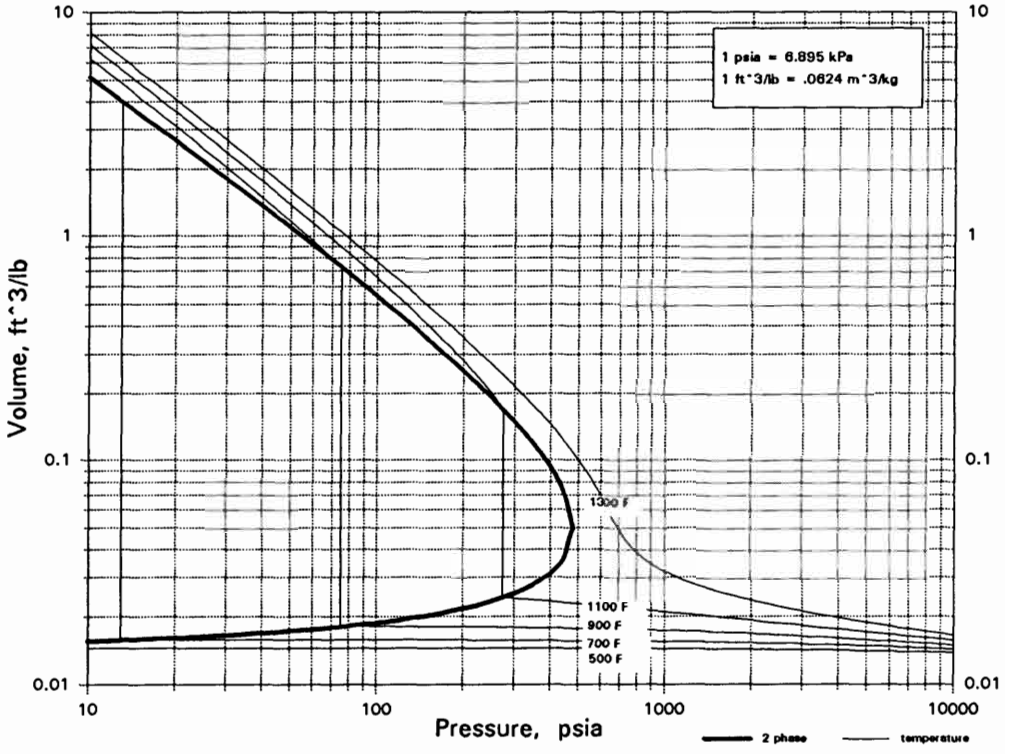


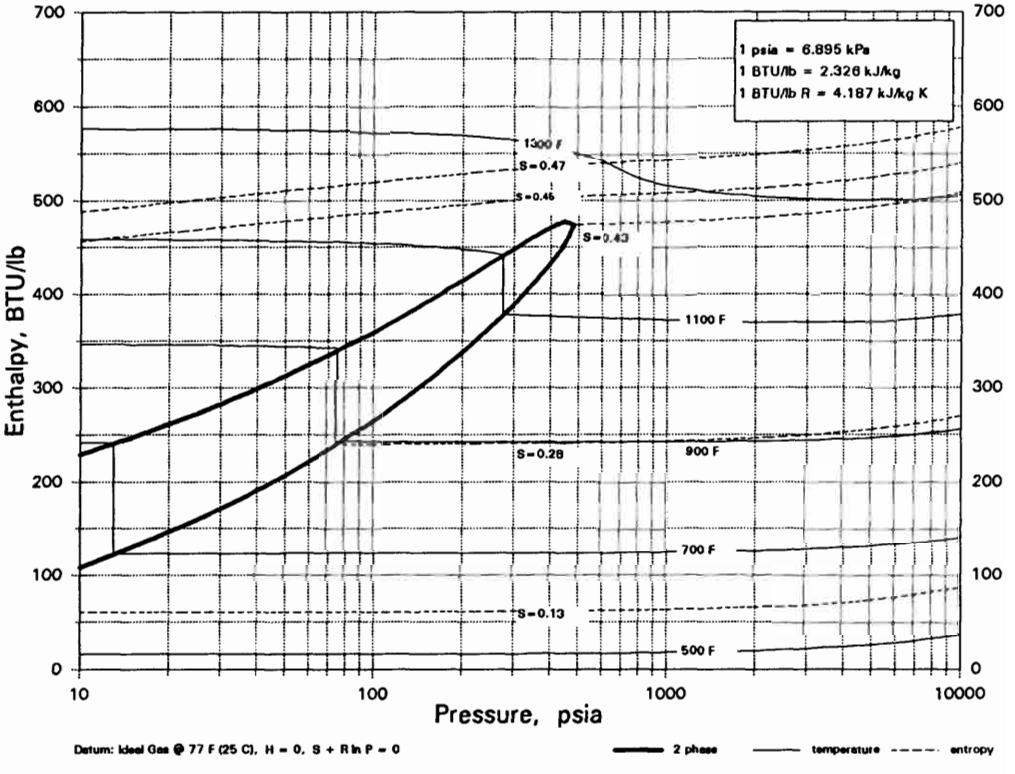
C18H14 o-TERPHENYL



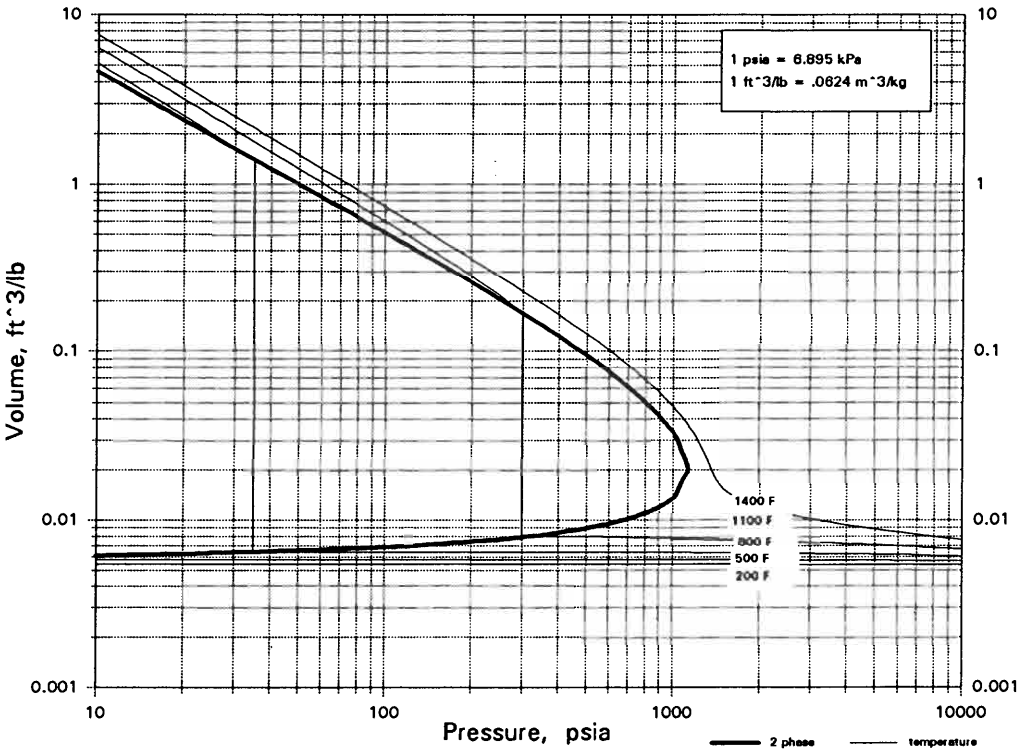


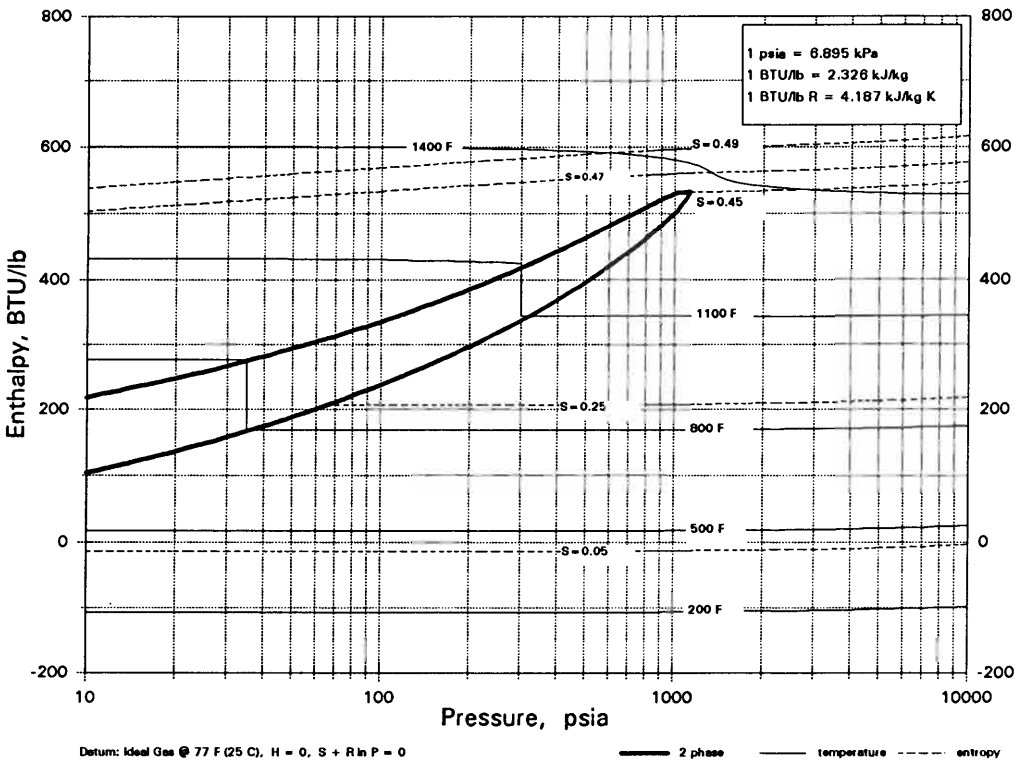
C18H14 p-TERPHENYL





C18H15P TRIPHENYLPHOSPHINE





C18H15O4P TRIPHENYL PHOSPHATE

1. Molecular Weight, lb/mol..... 326.29

2. Boiling Point, K..... 686.65

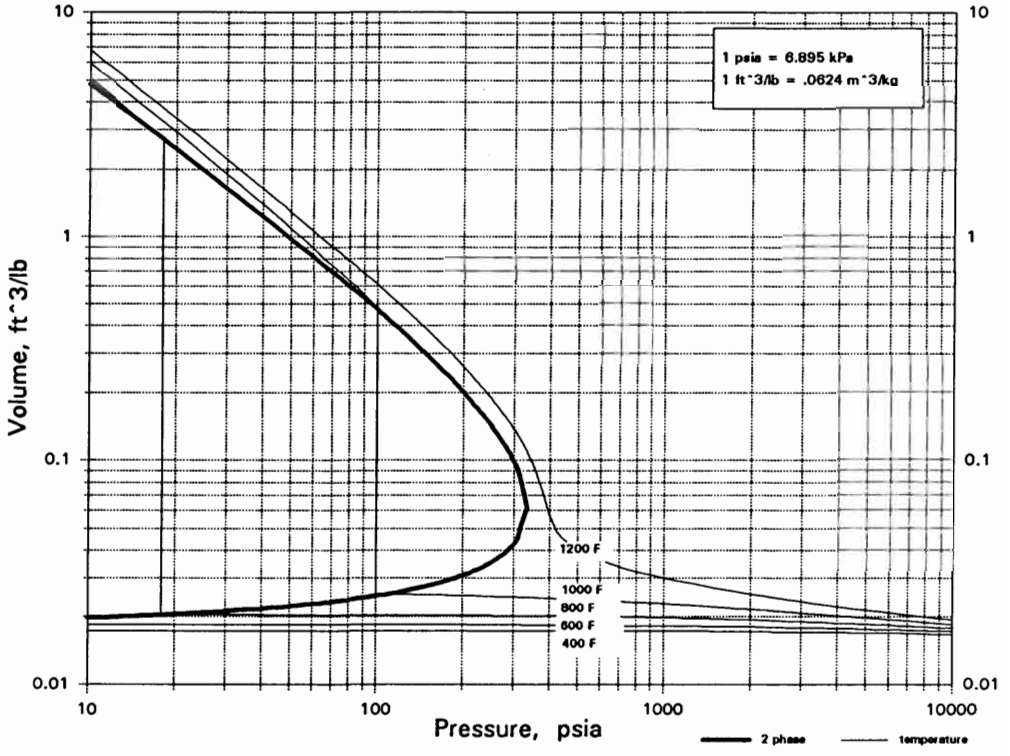
Critical data (Tc, Pc) are not available.

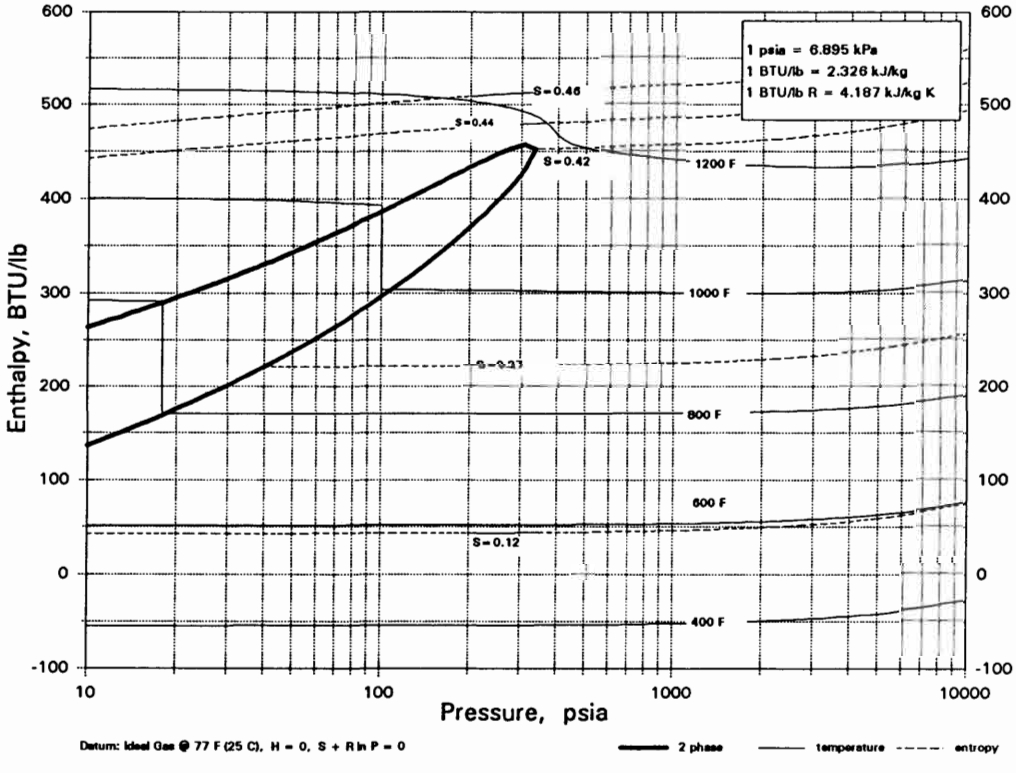
1. Molecular Weight, lb/mol..... 326.29

2. Boiling Point, K..... 686.65

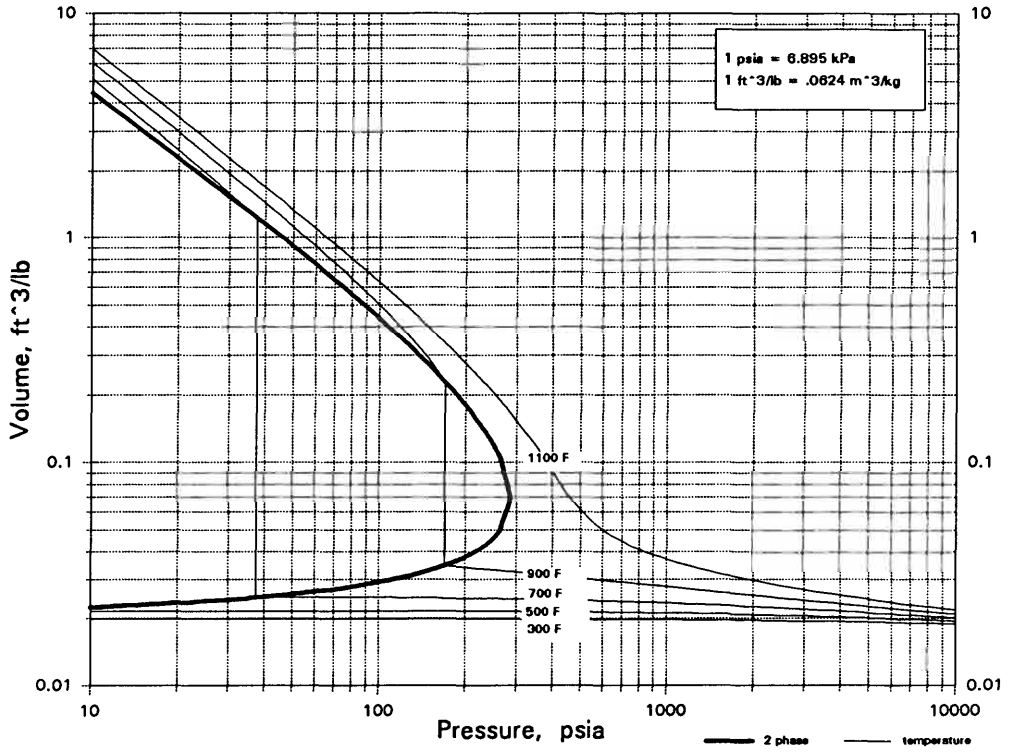
Critical data (Tc, Pc) are not available.

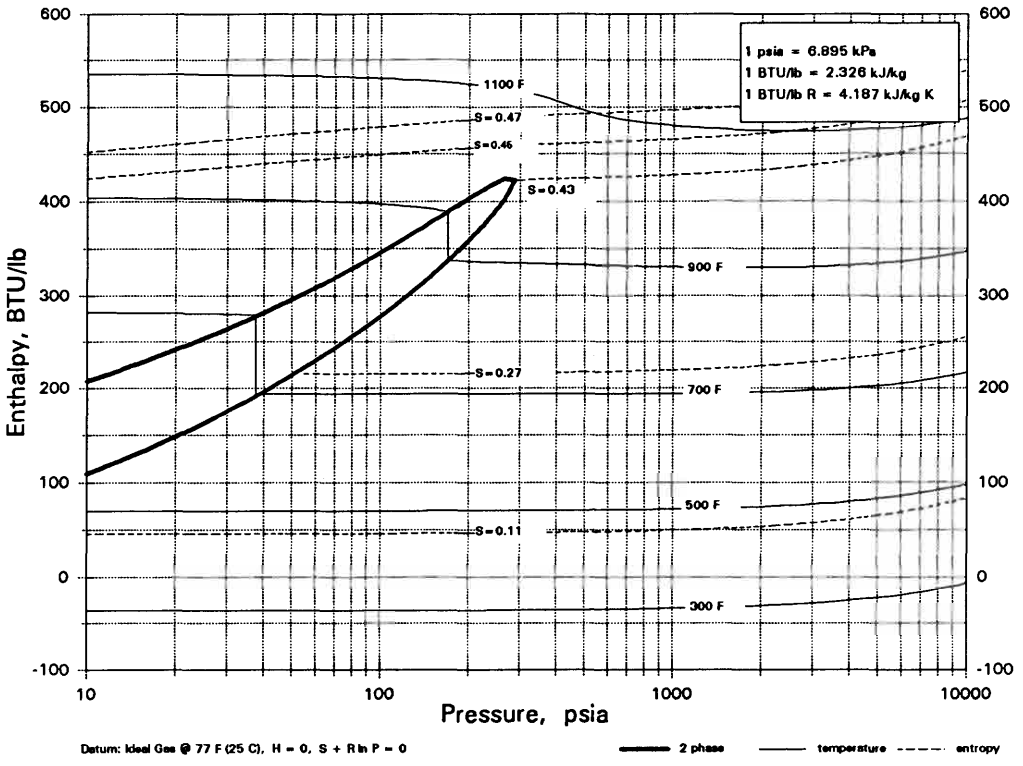
C18H16N2 N-N'-DIPHENYL-p-PHENYLENEDIAMINE



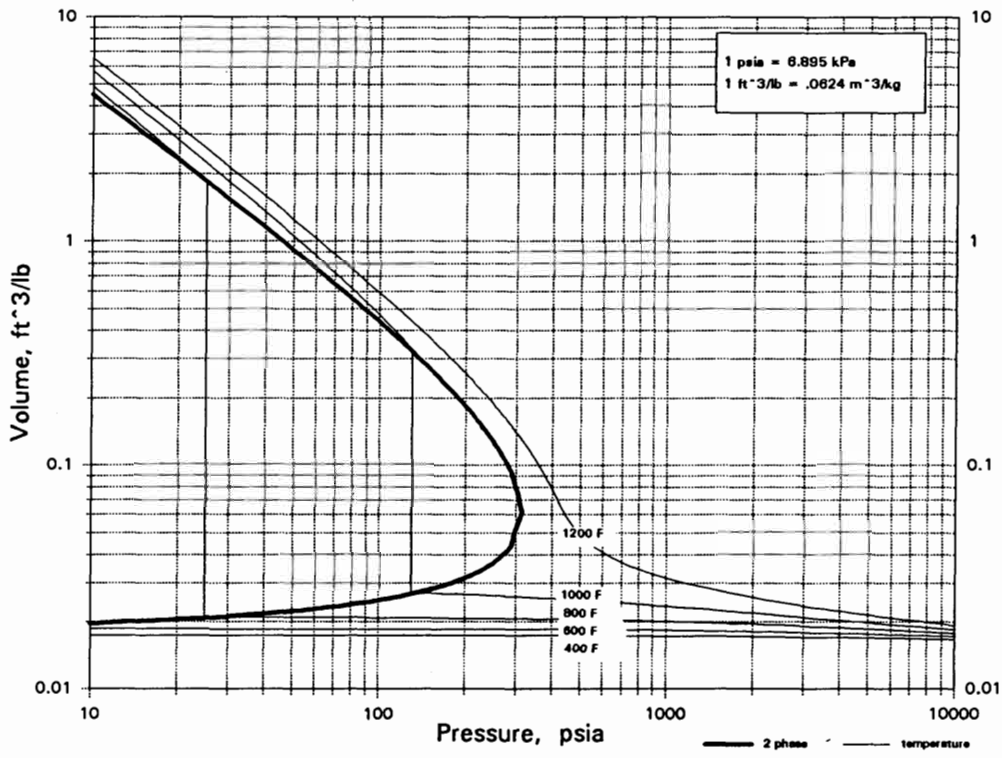


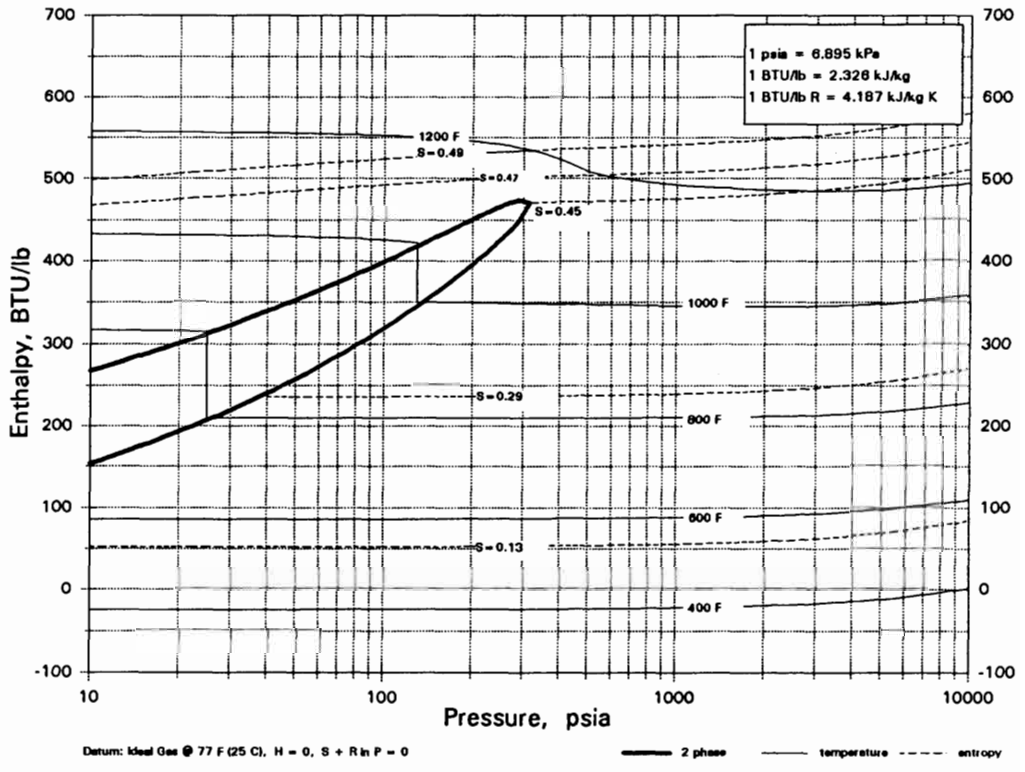
C18H22 2-3-DIMETHYL-2-3-DIPHENYLBUTANE



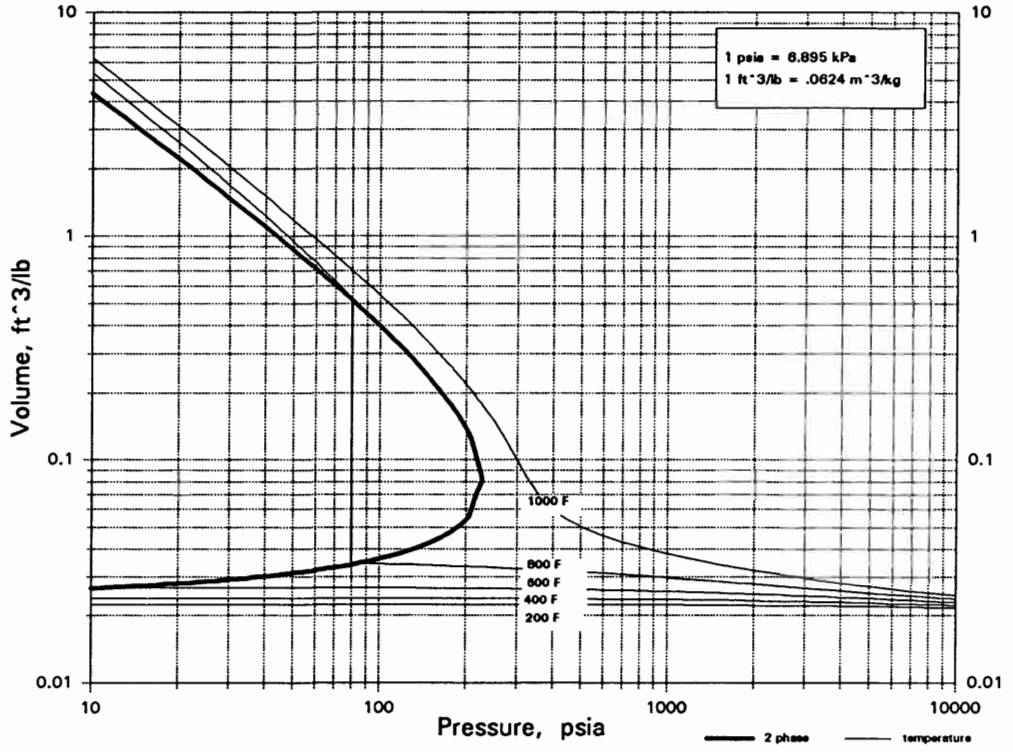


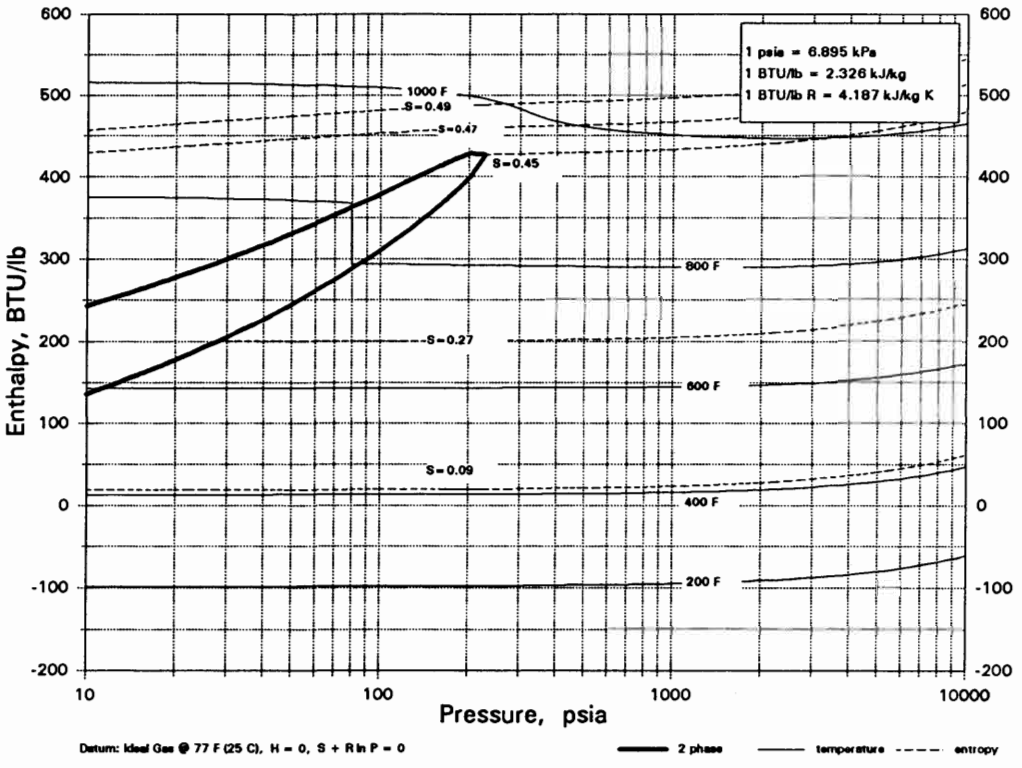
C18H22O2 DICUMYL PEROXIDE



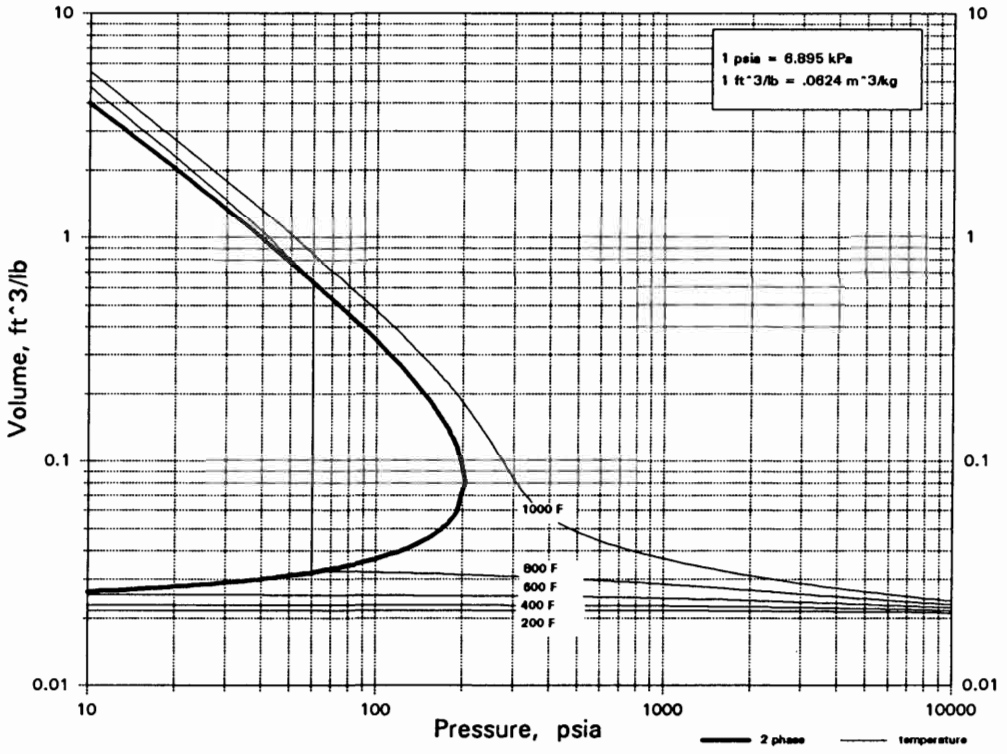


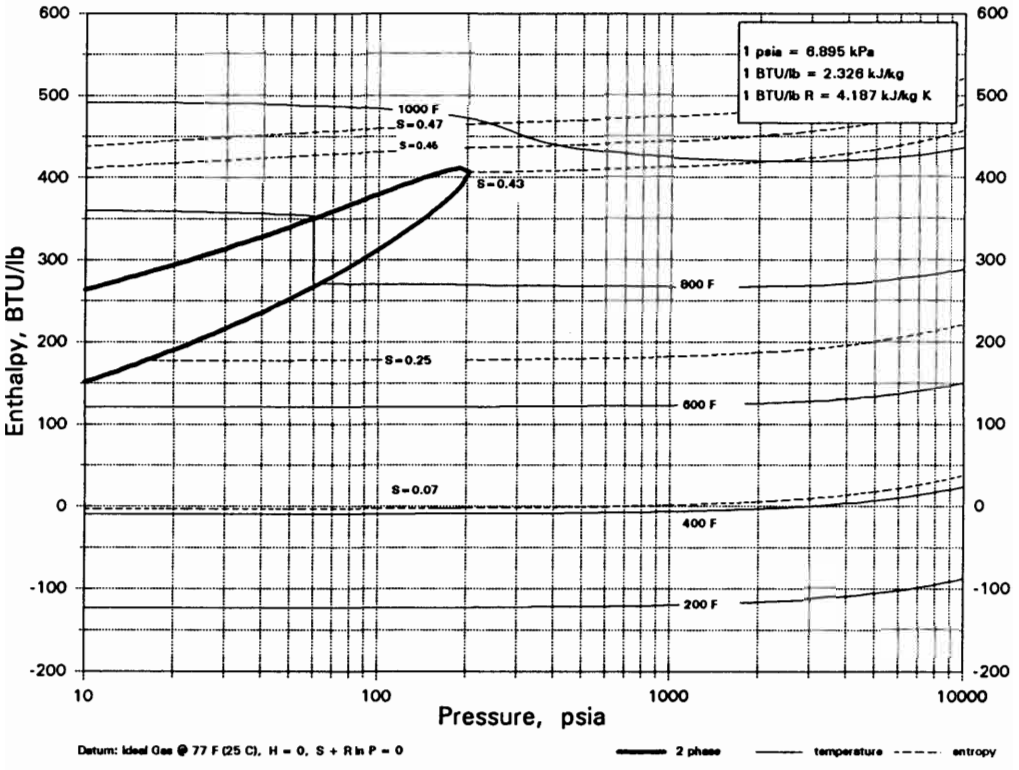
C18H30 n-DODECYLBENZENE



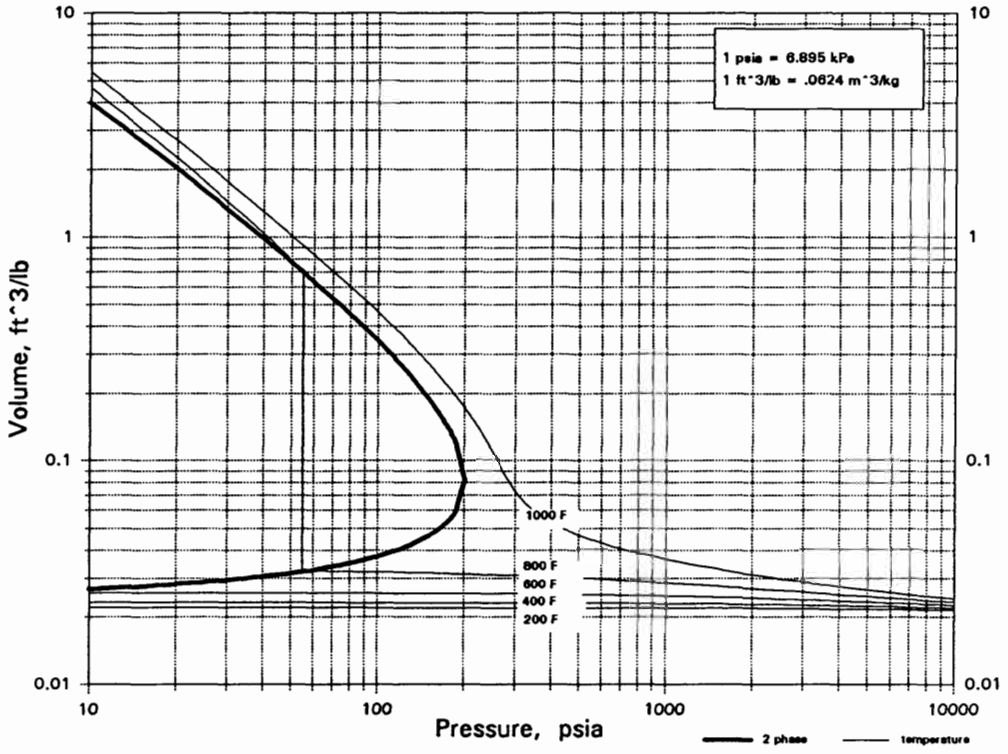


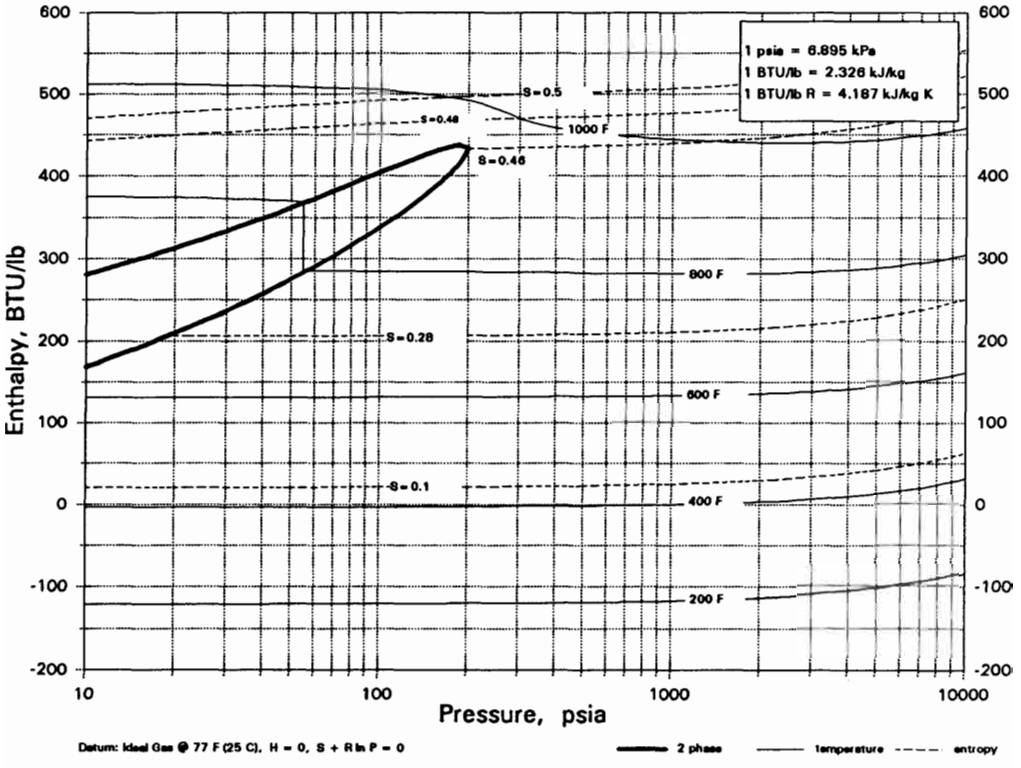
C18H32O2 LINOLEIC ACID



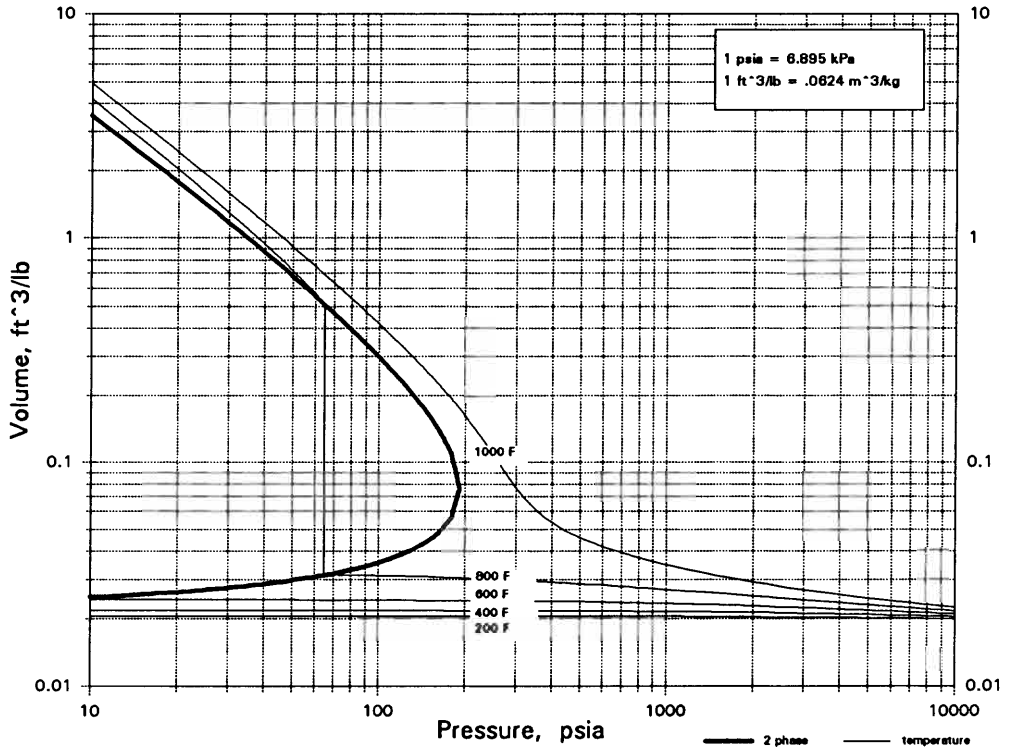


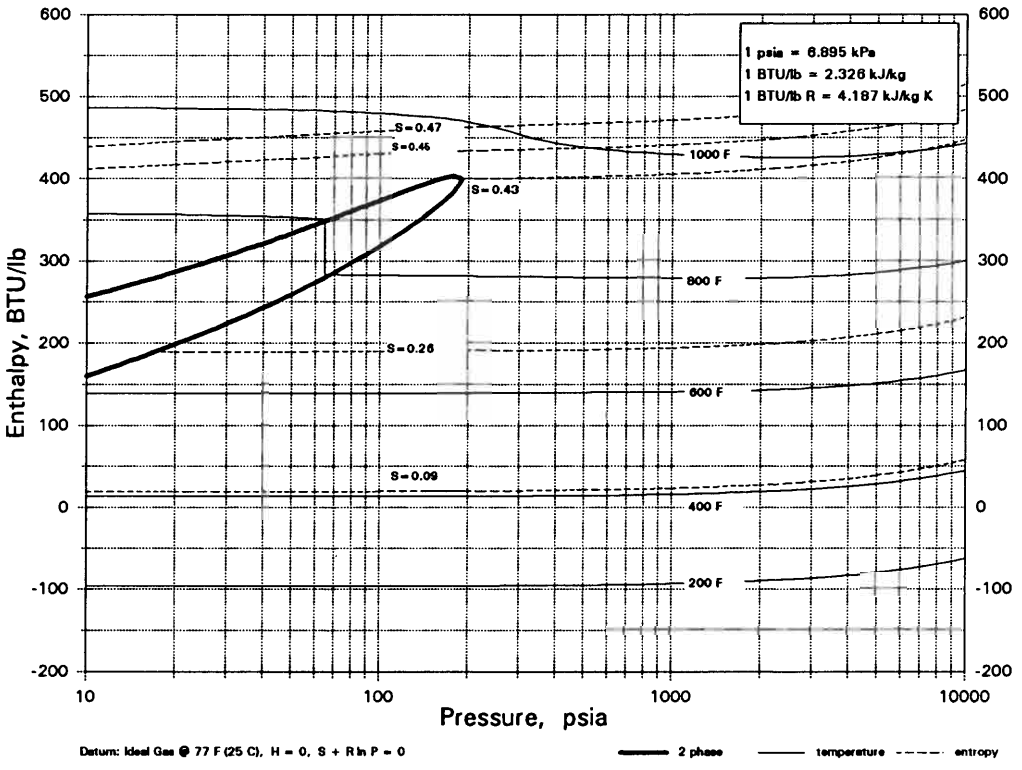
C18H34O2 OLEIC ACID





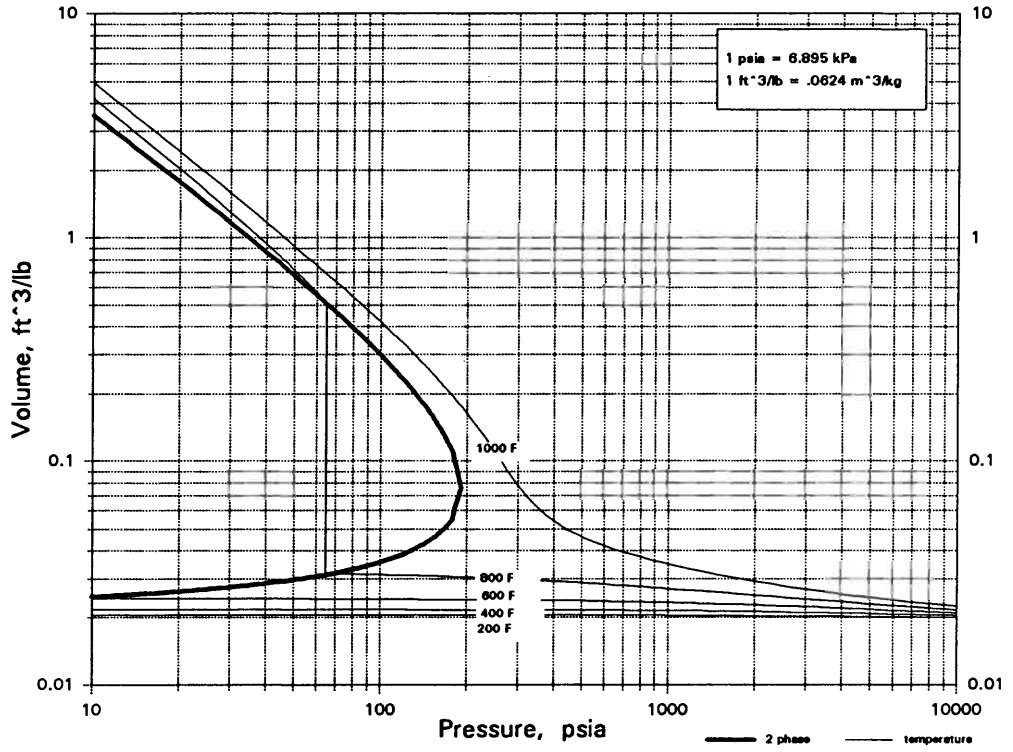
C18H34O4 DIBUTYL SEBACATE

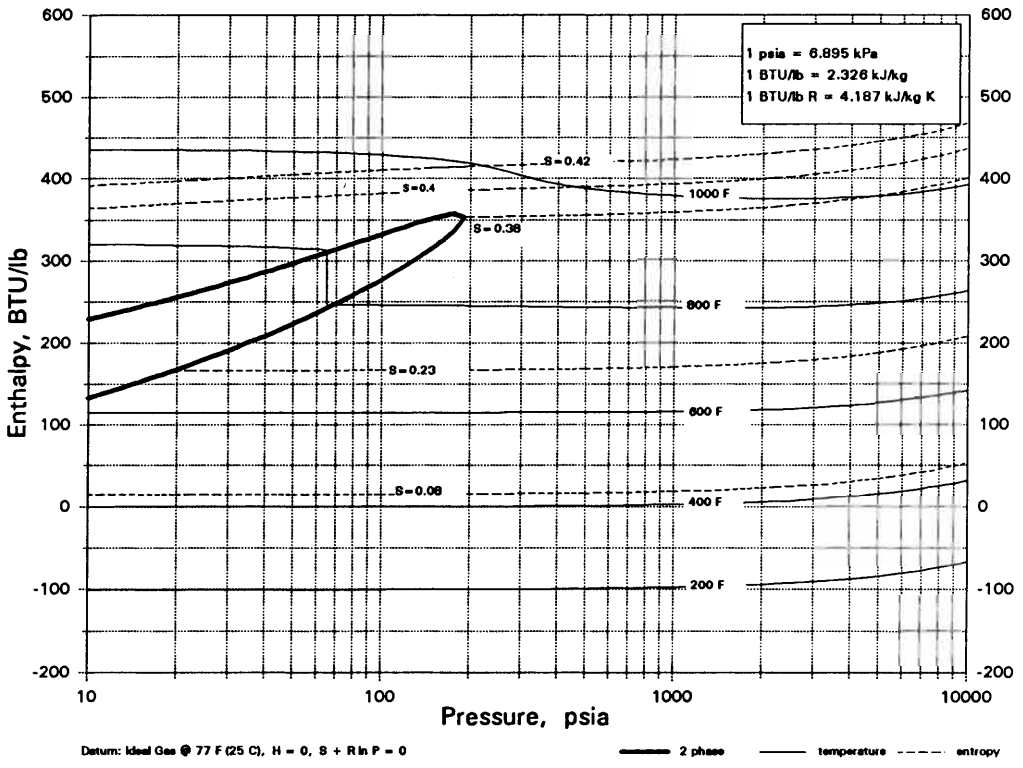




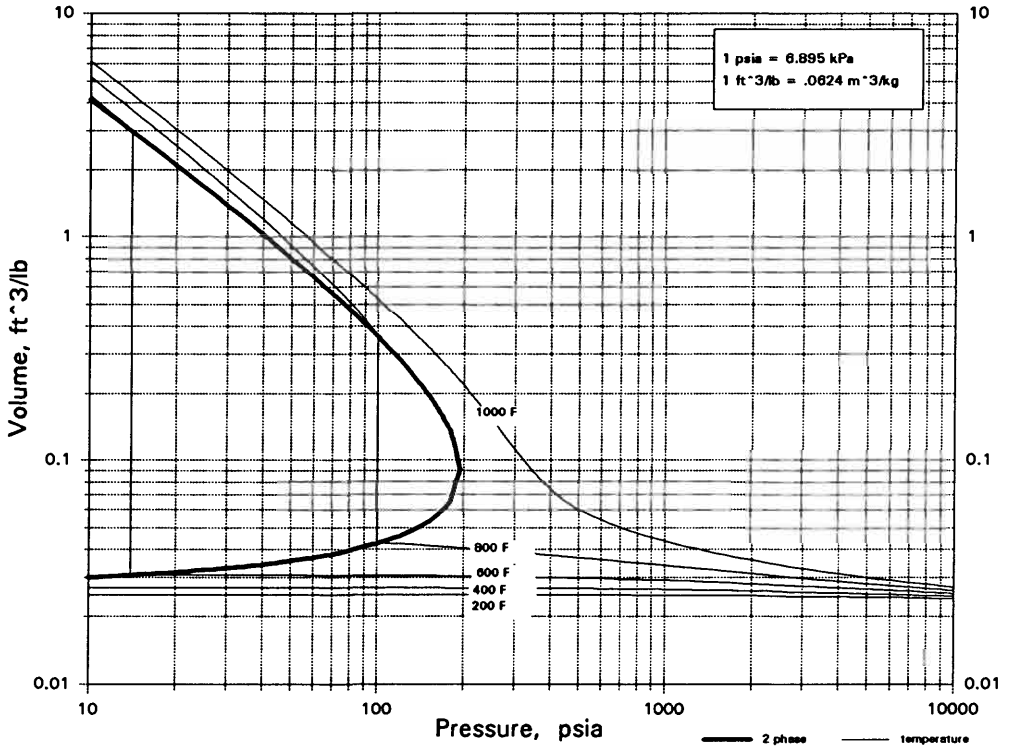
Datum: Ideal Gas @ 77 F (25 C), H = 0, S + R ln P = 0

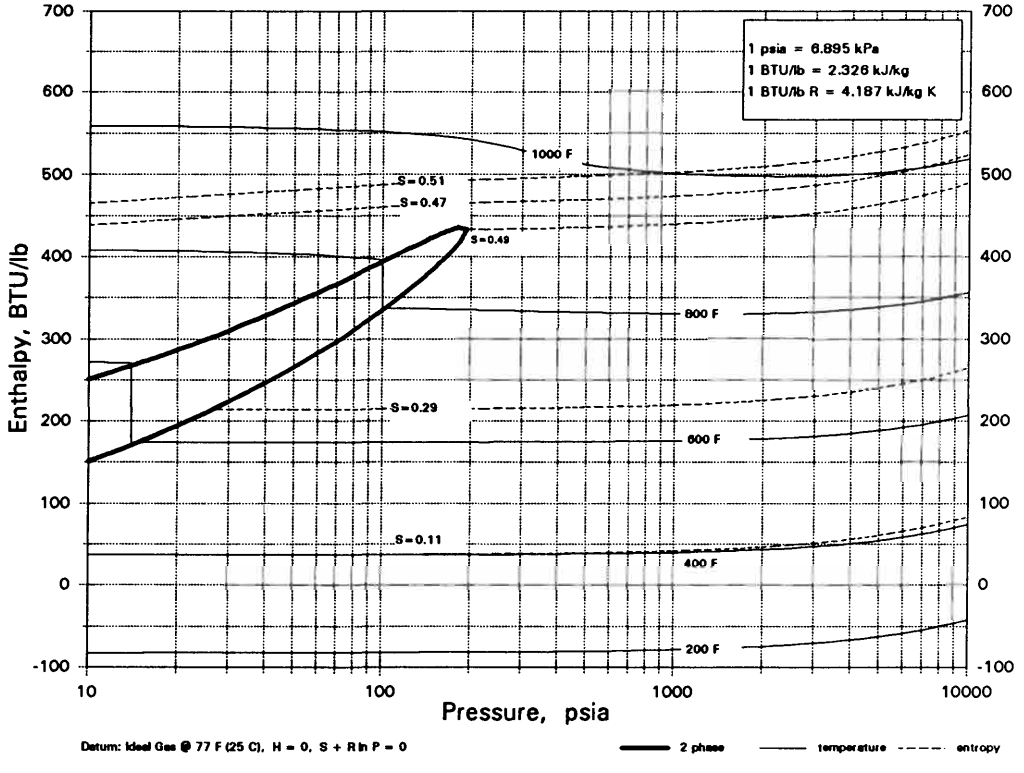
C18H34O4 DIHEXYL ADIPATE



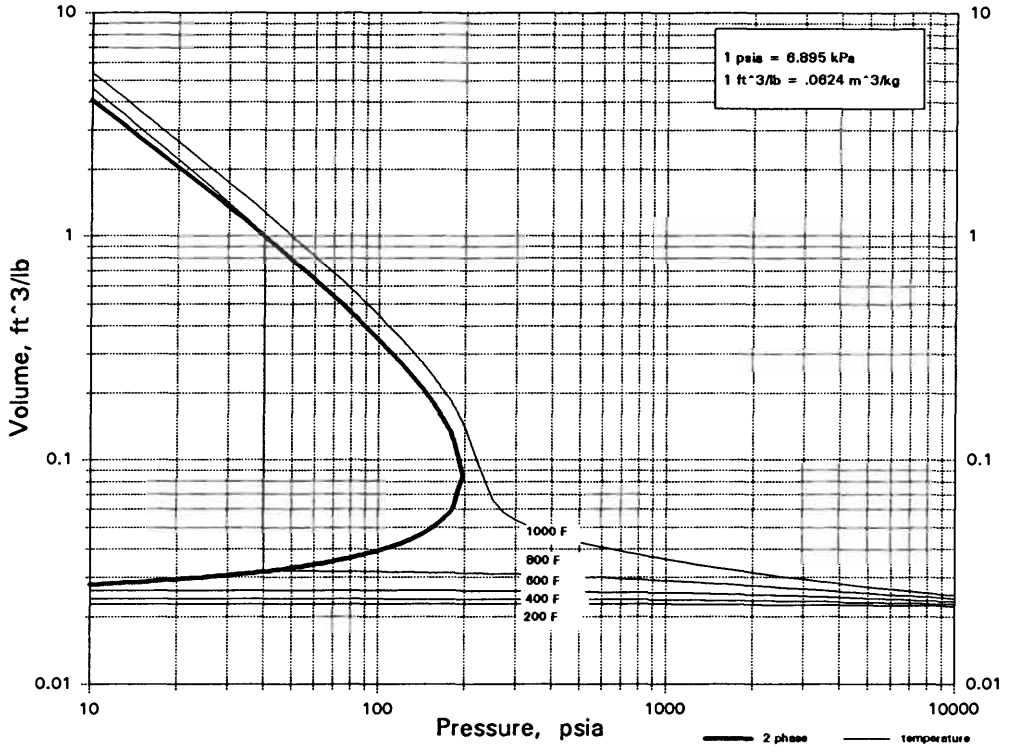


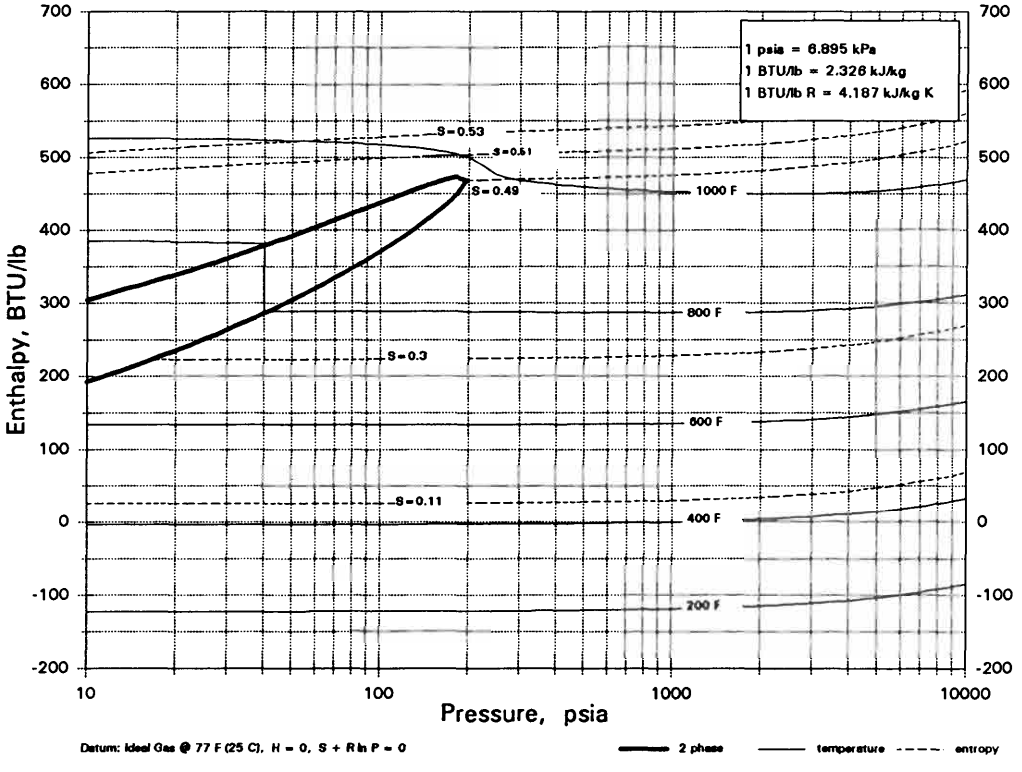
C18H36 1-OCTADECENE



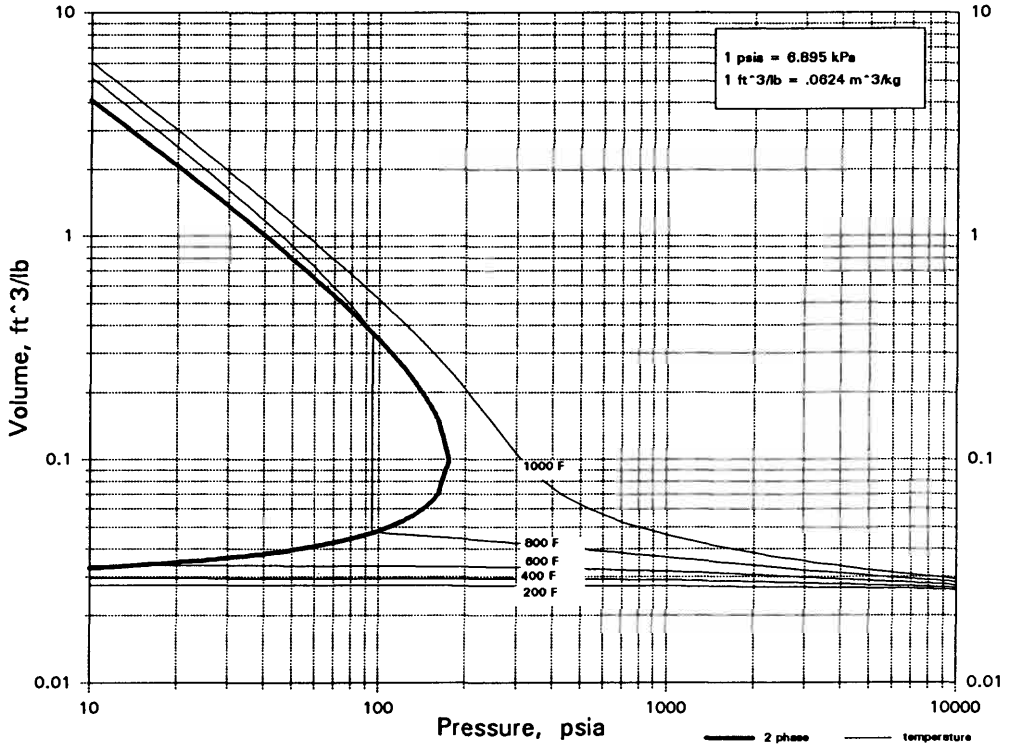


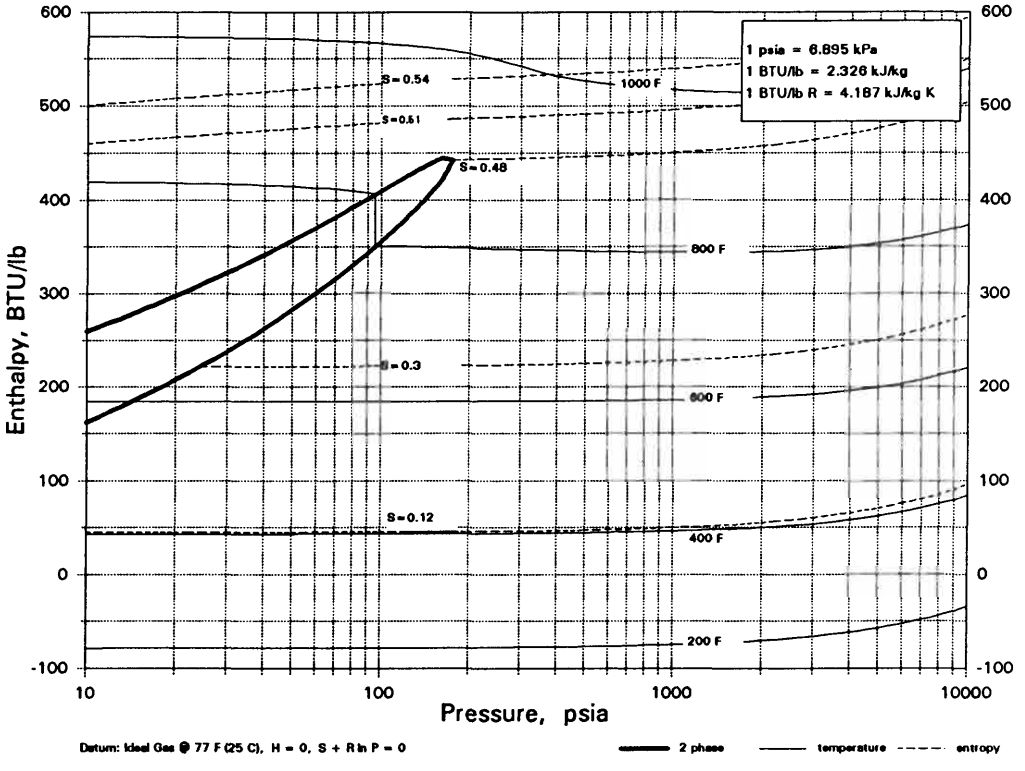
C18H36O2 STEARIC ACID



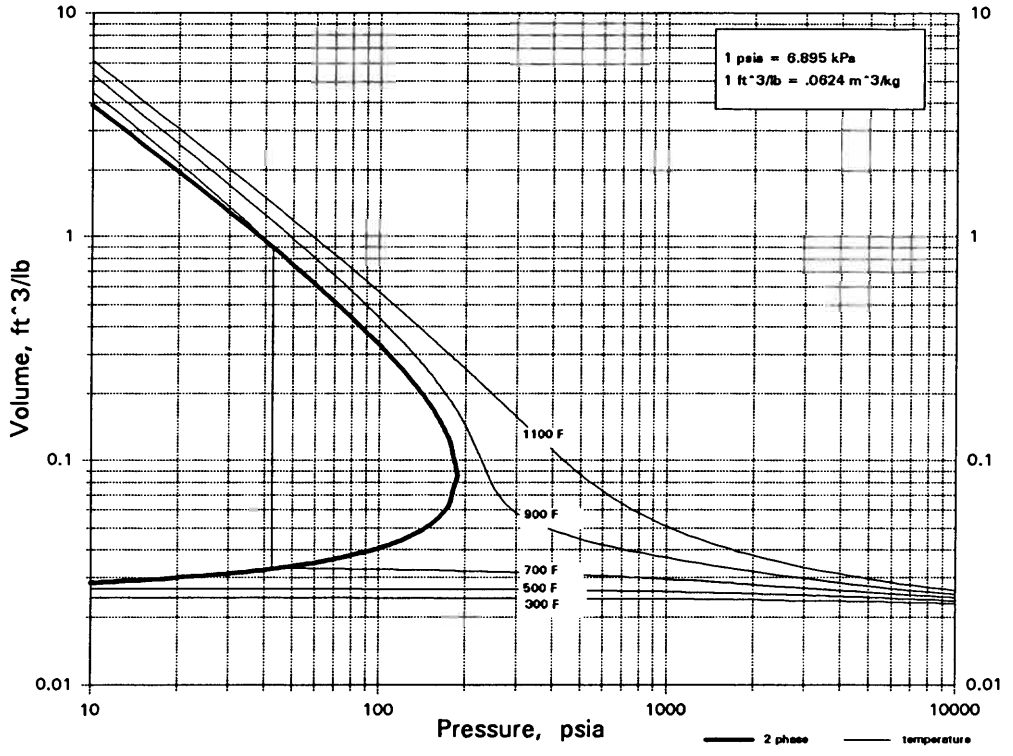


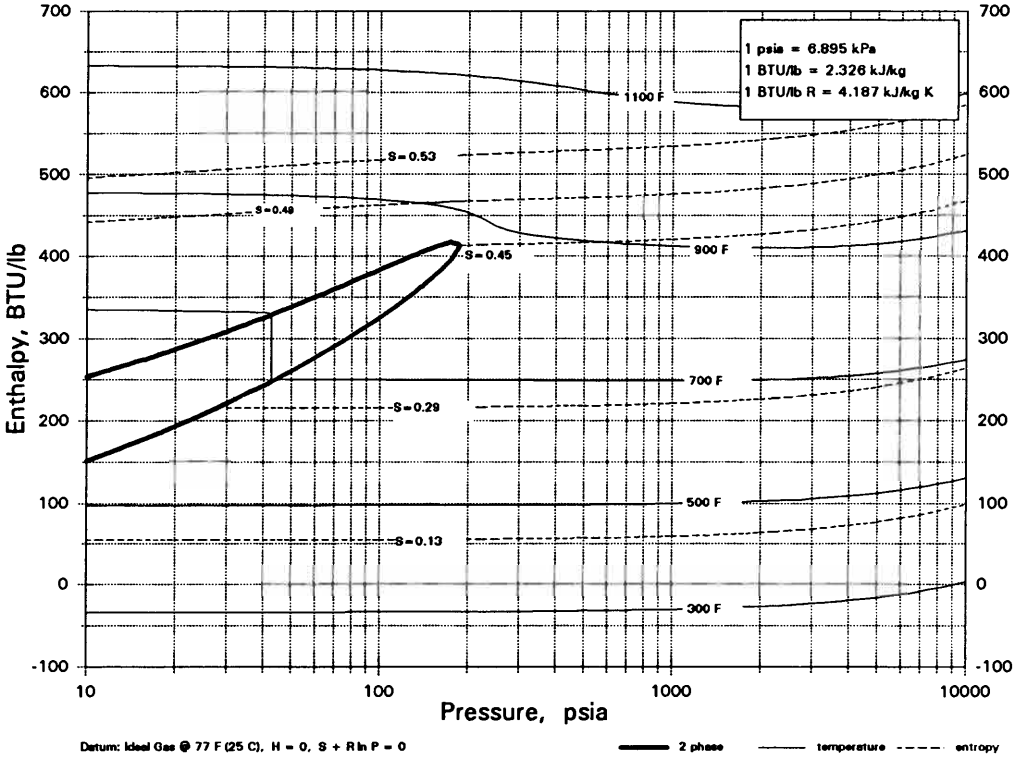
C18H38 n-OCTADECANE



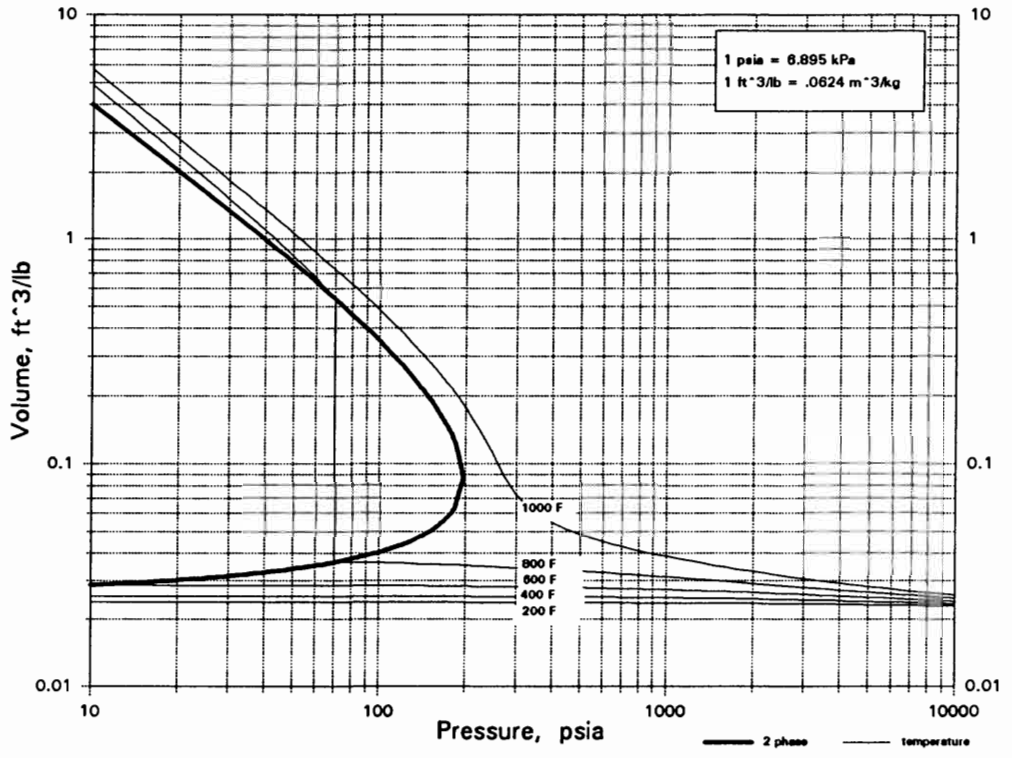


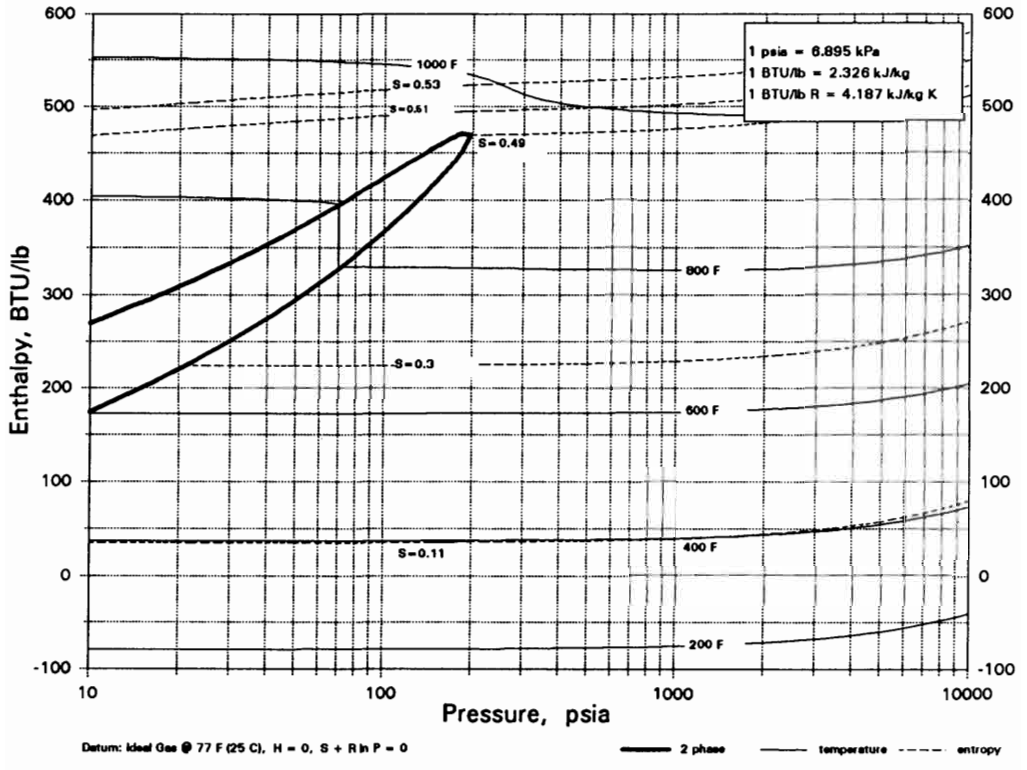
C18H38O DINONYL ETHER



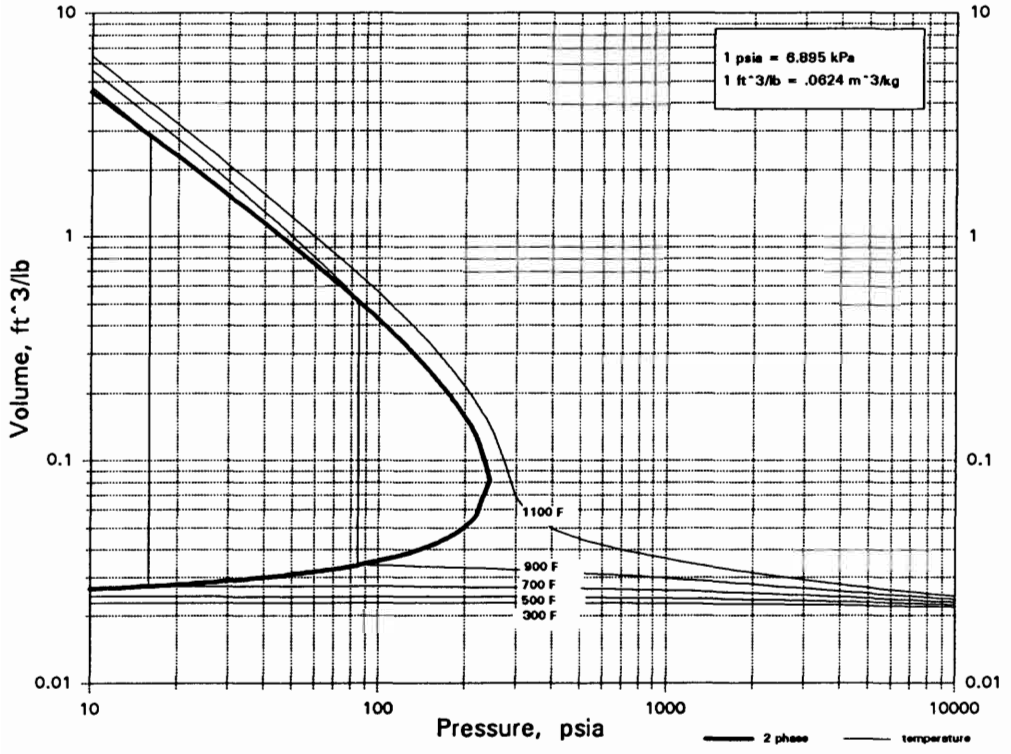


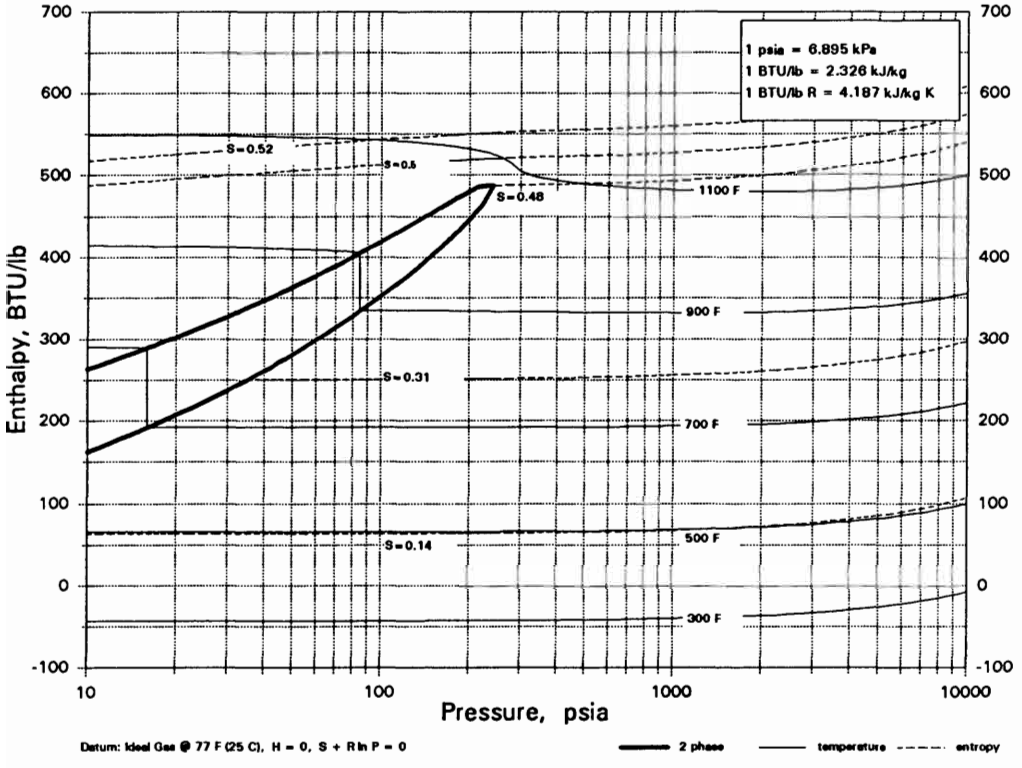
C18H38O 1-OCTADECANOL



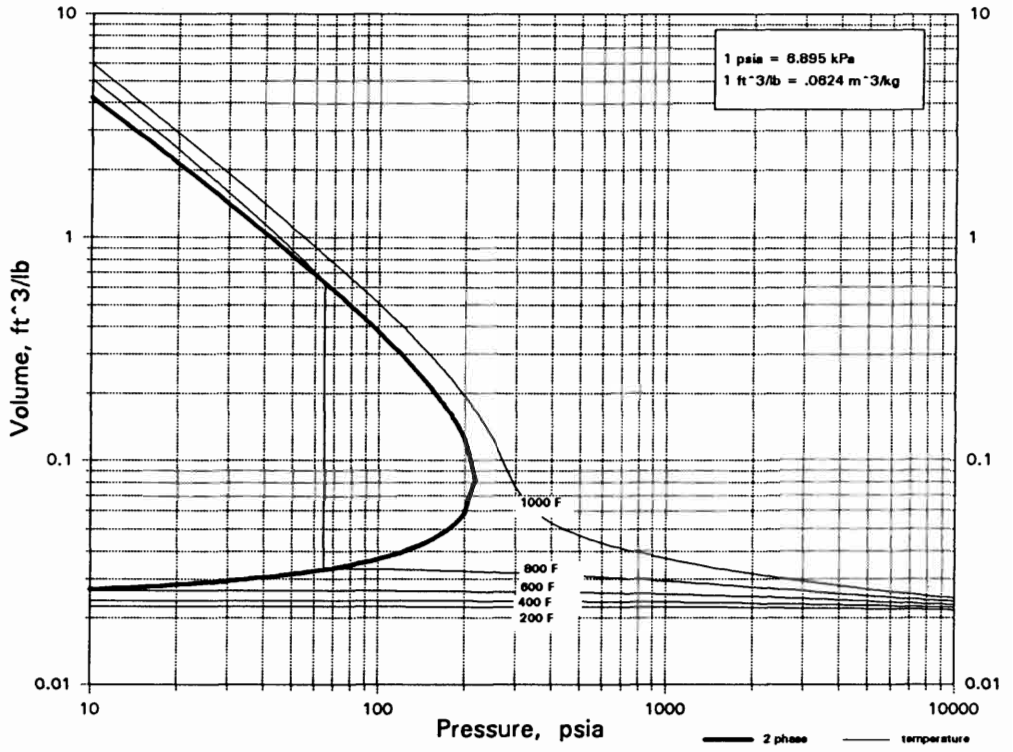


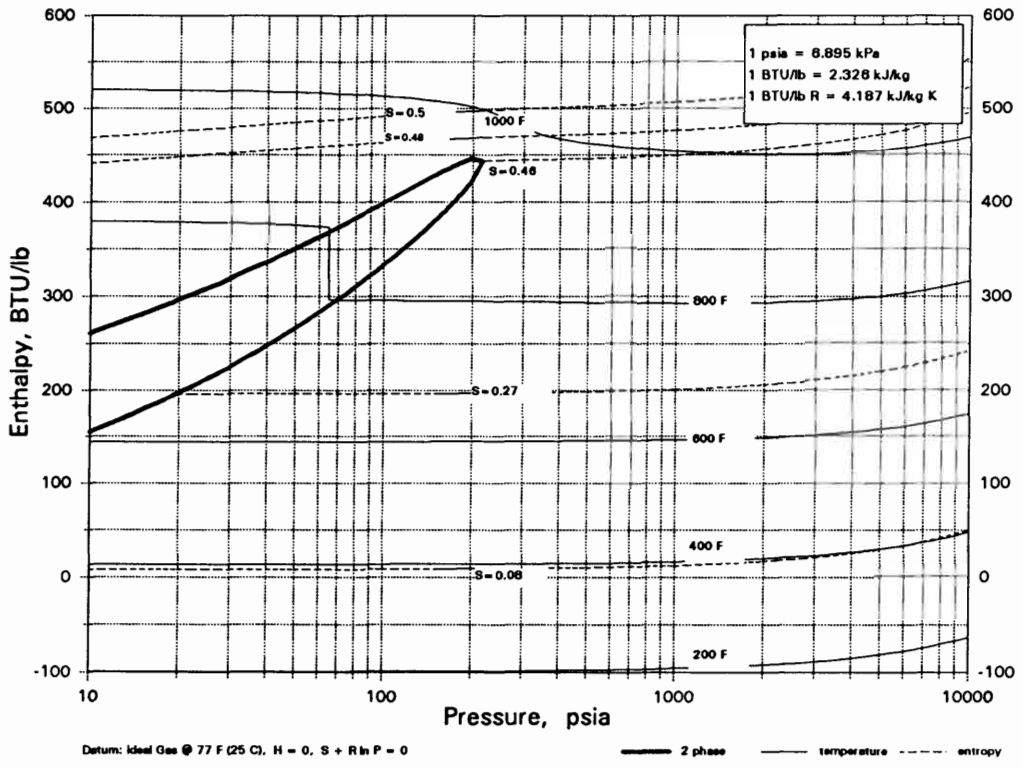
C19H26 1-n-NONYLNAPHTHALENE



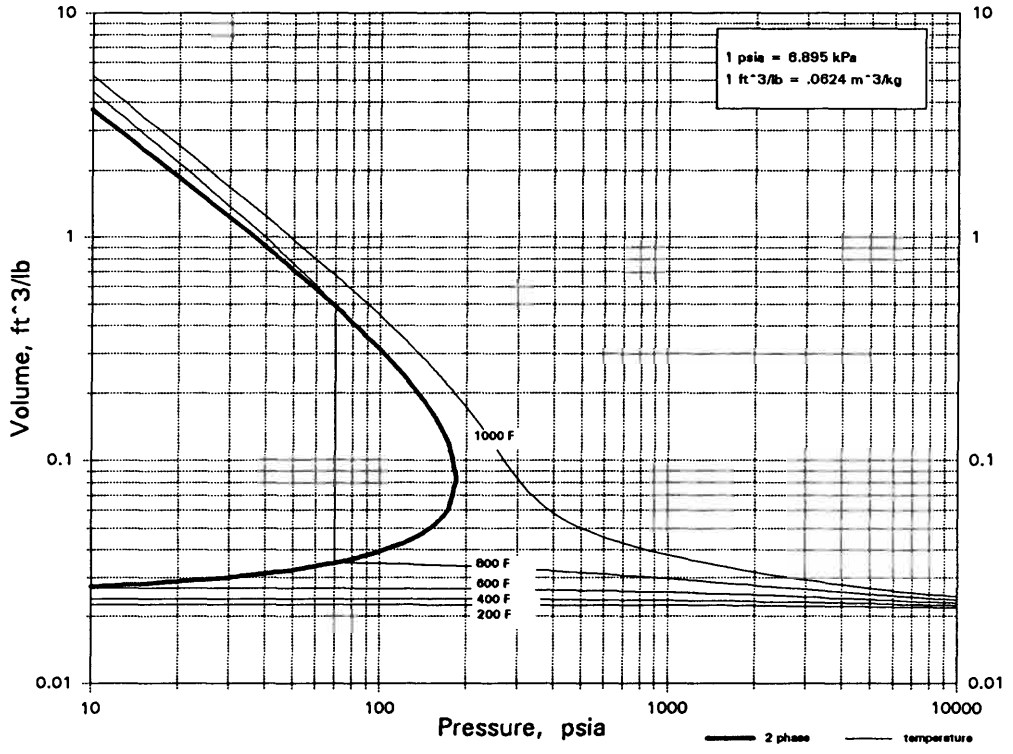


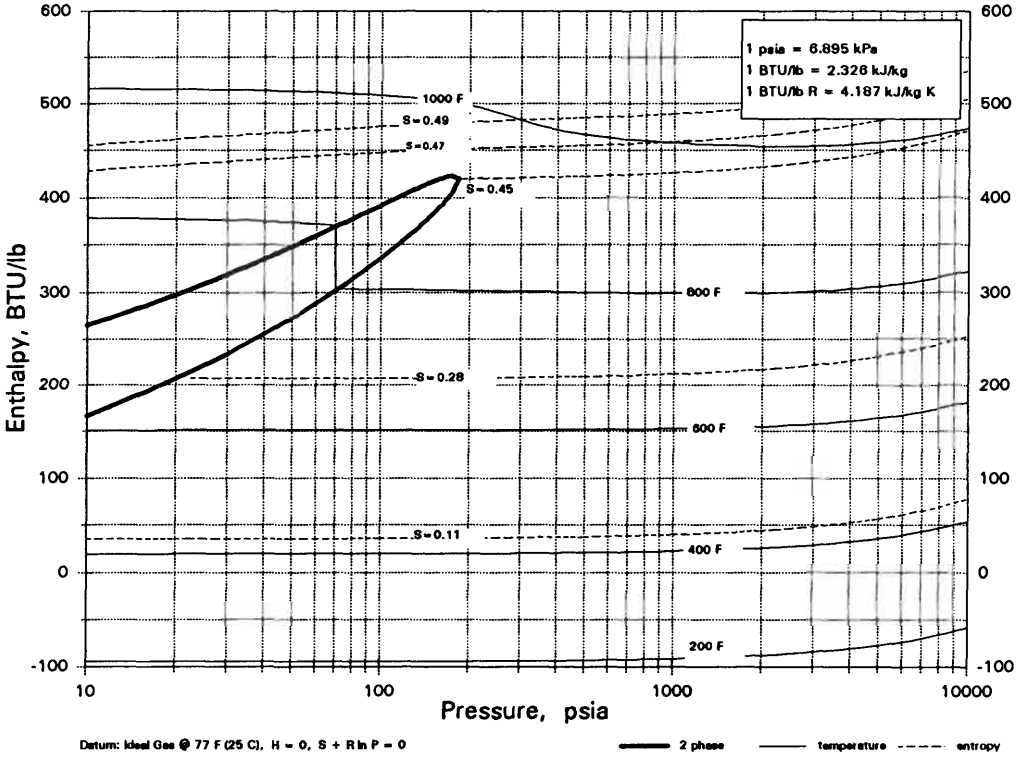
C19H32 n-TRIDECYLBENZENE



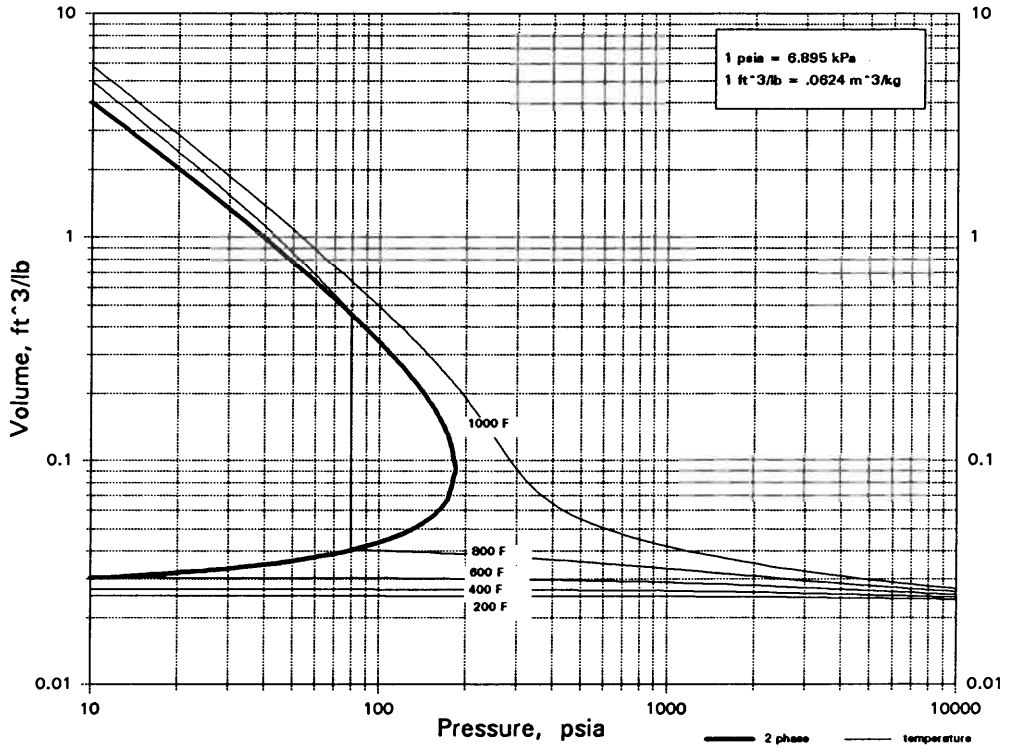


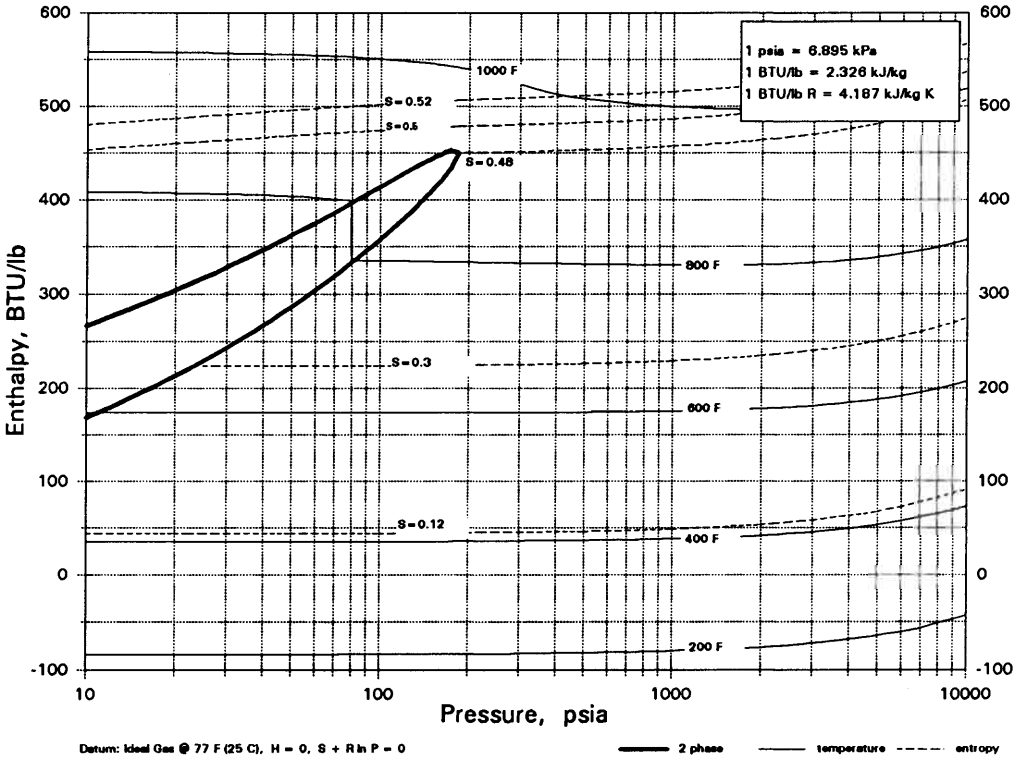
C19H36O2 METHYL OLEATE



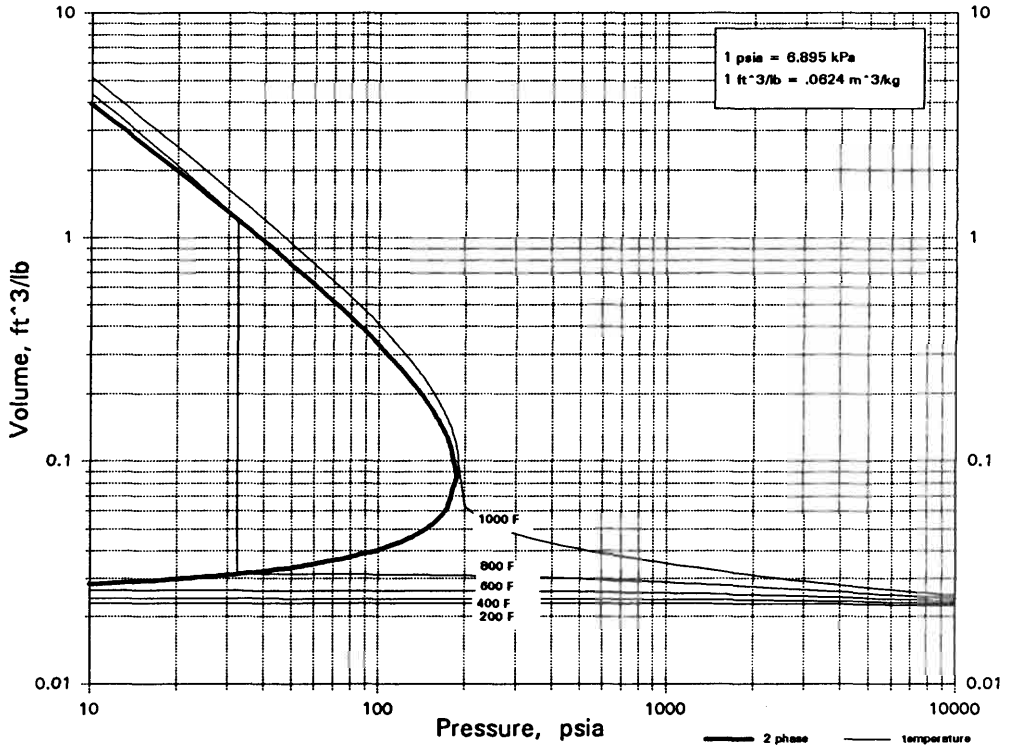


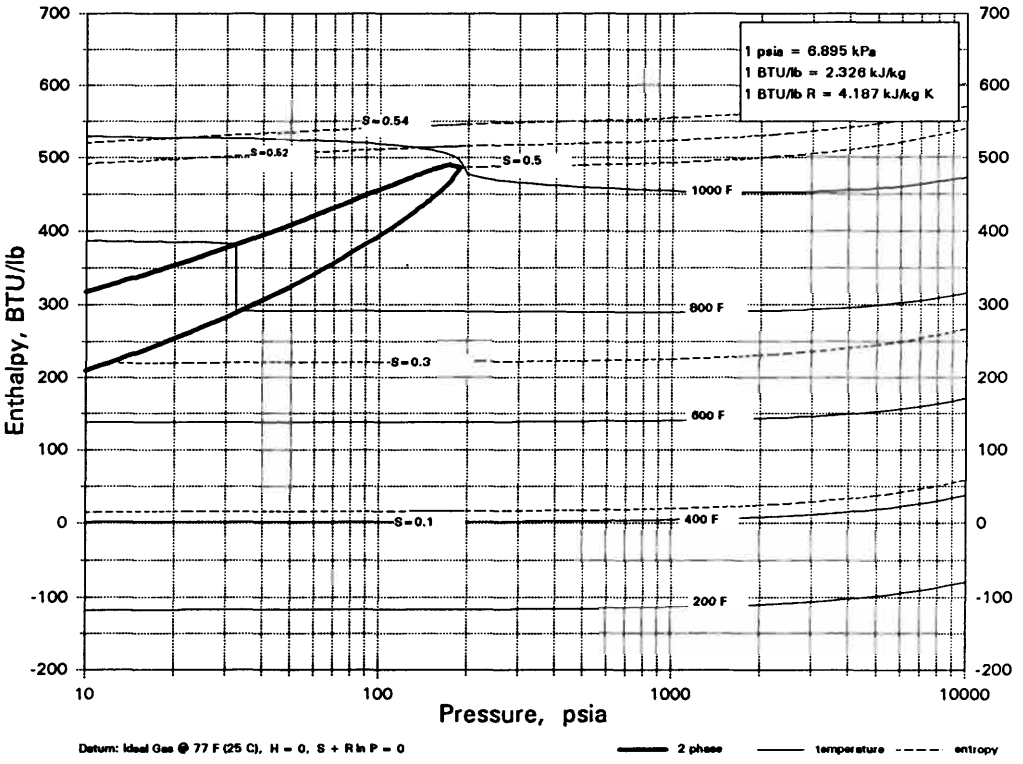
C19H38 1-NONADECENE



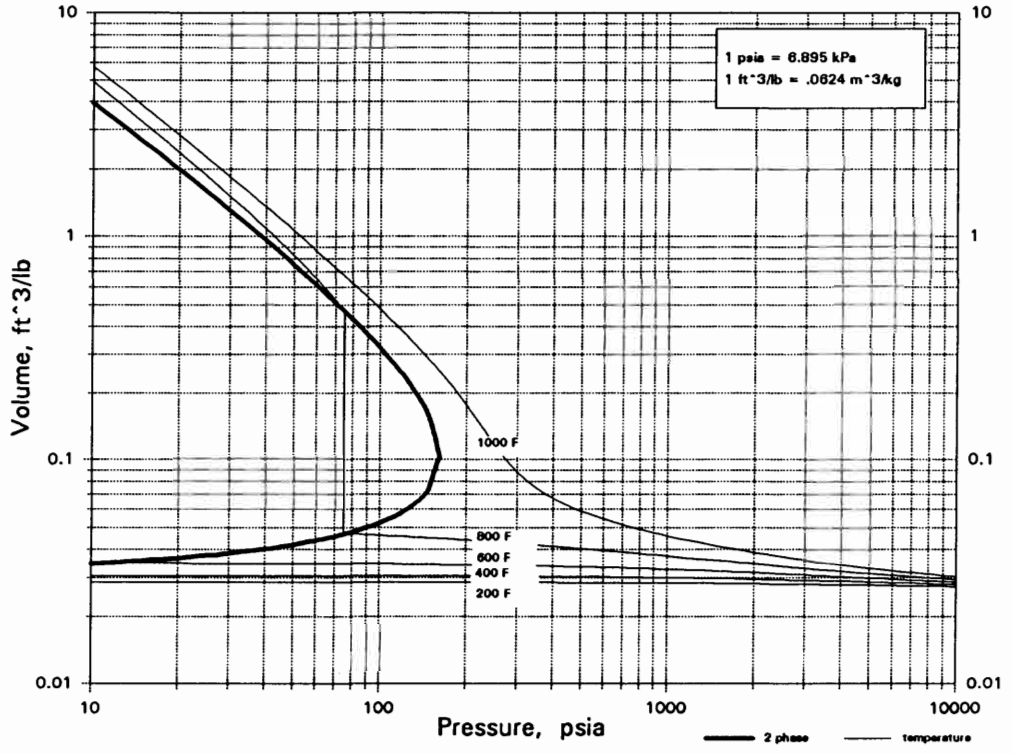


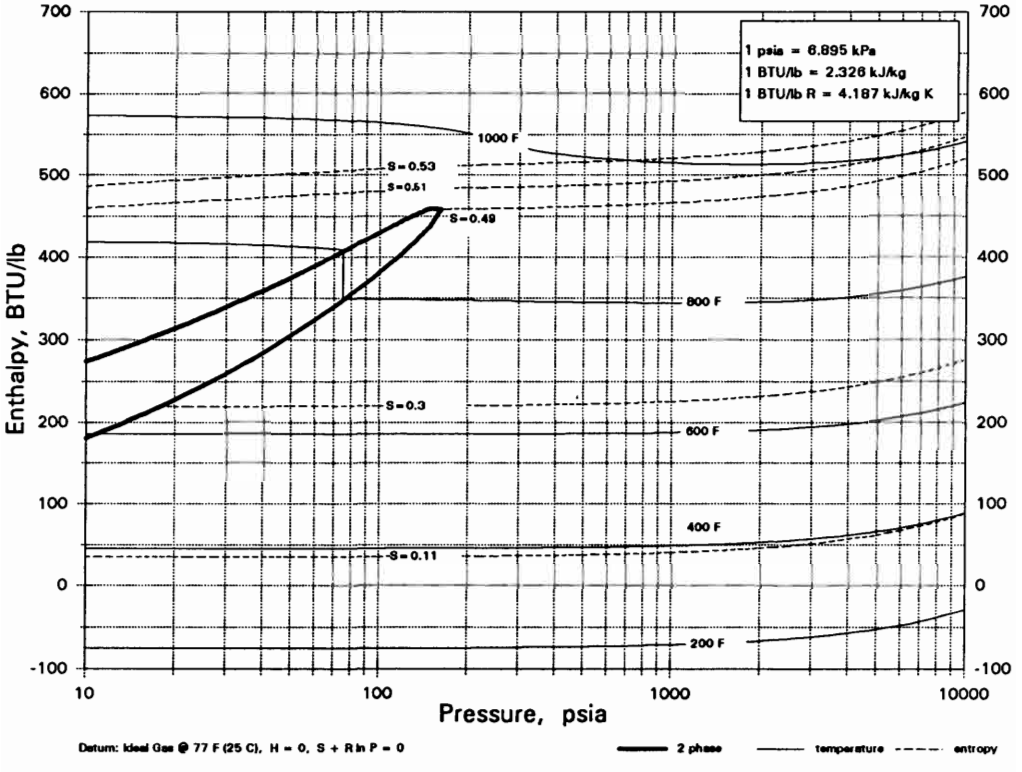
C19H38O2 NONADECANOIC ACID



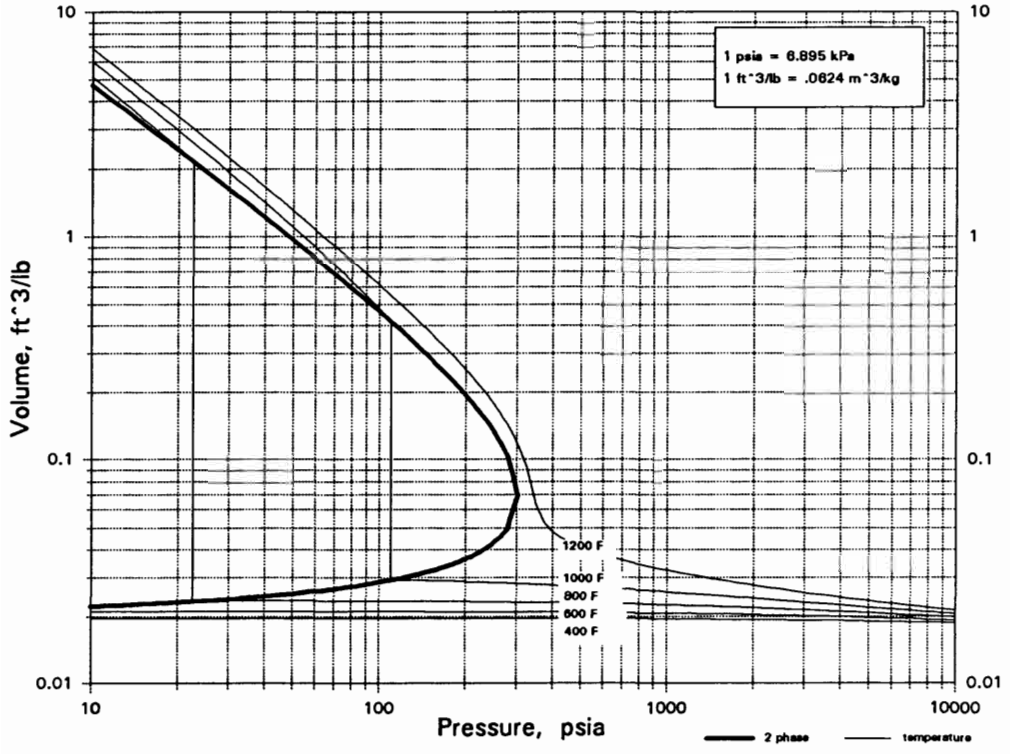


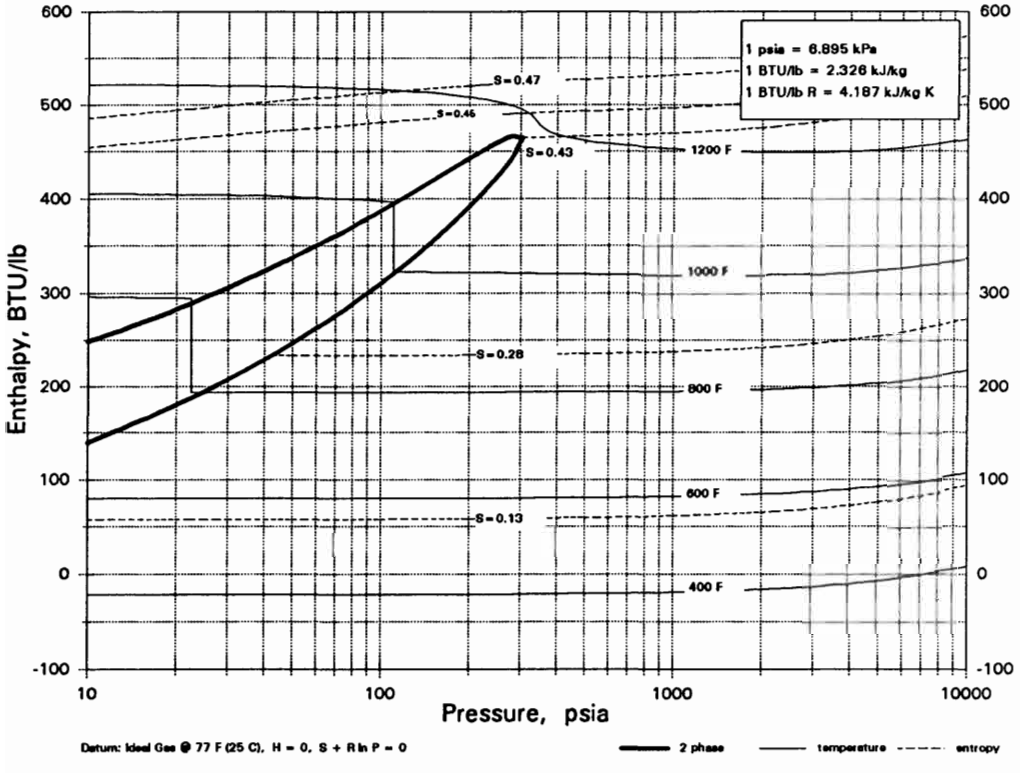
C19H40 n-NONADECANE



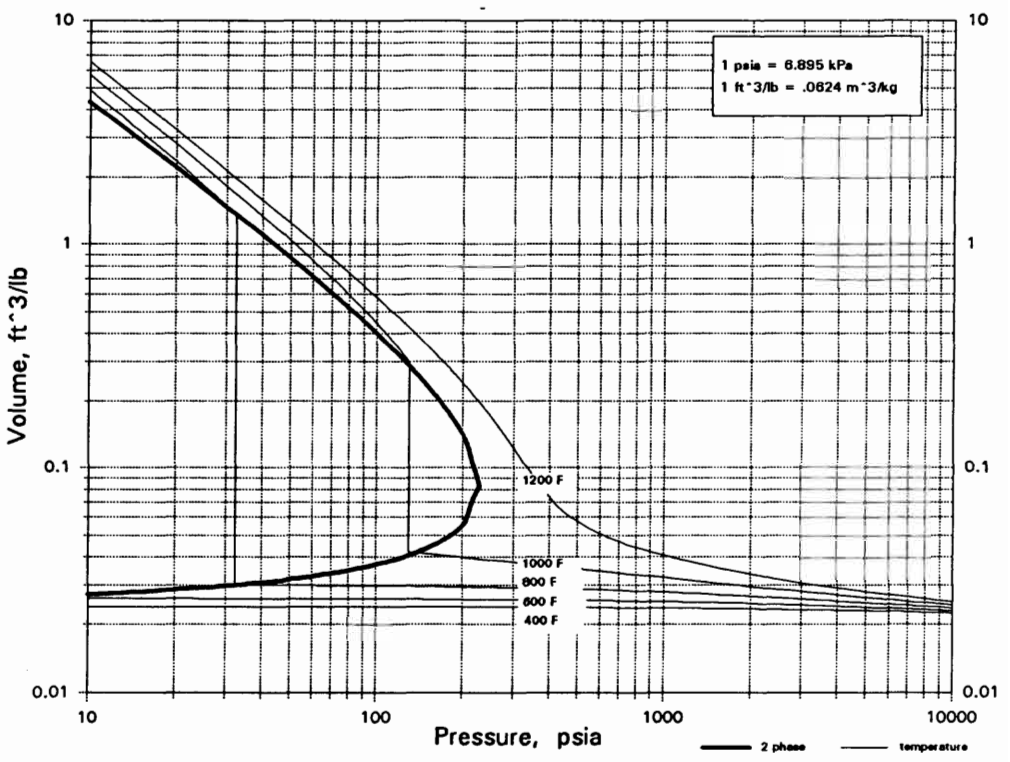


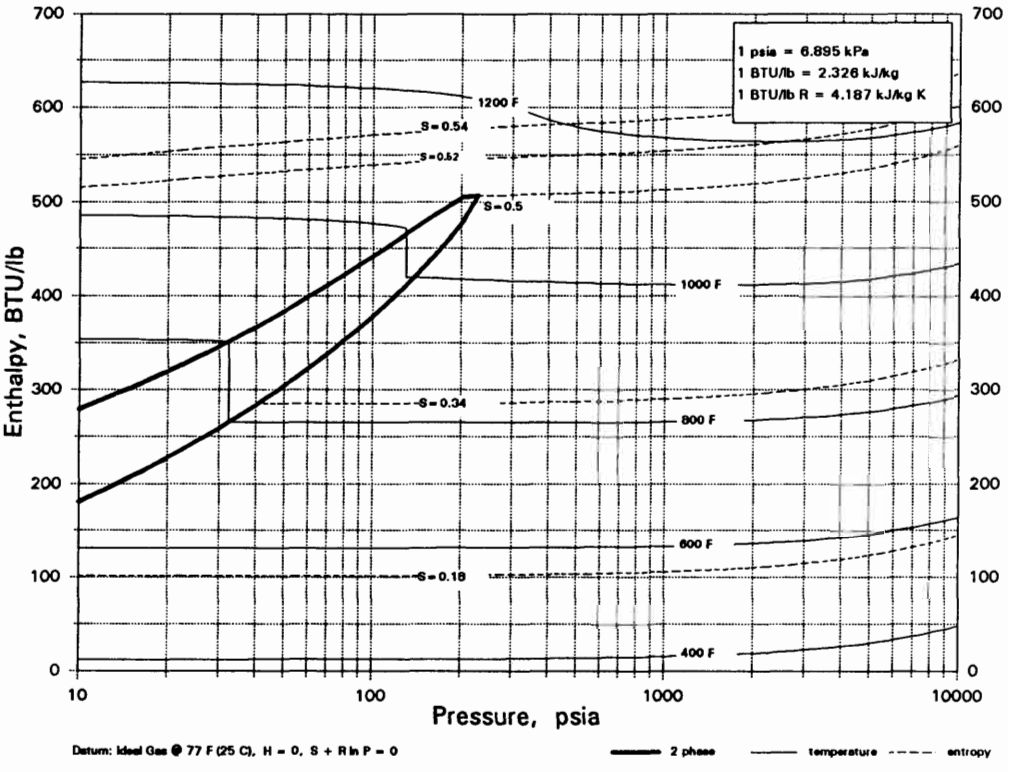
C20H16 TRIPHENYLETHYLENE



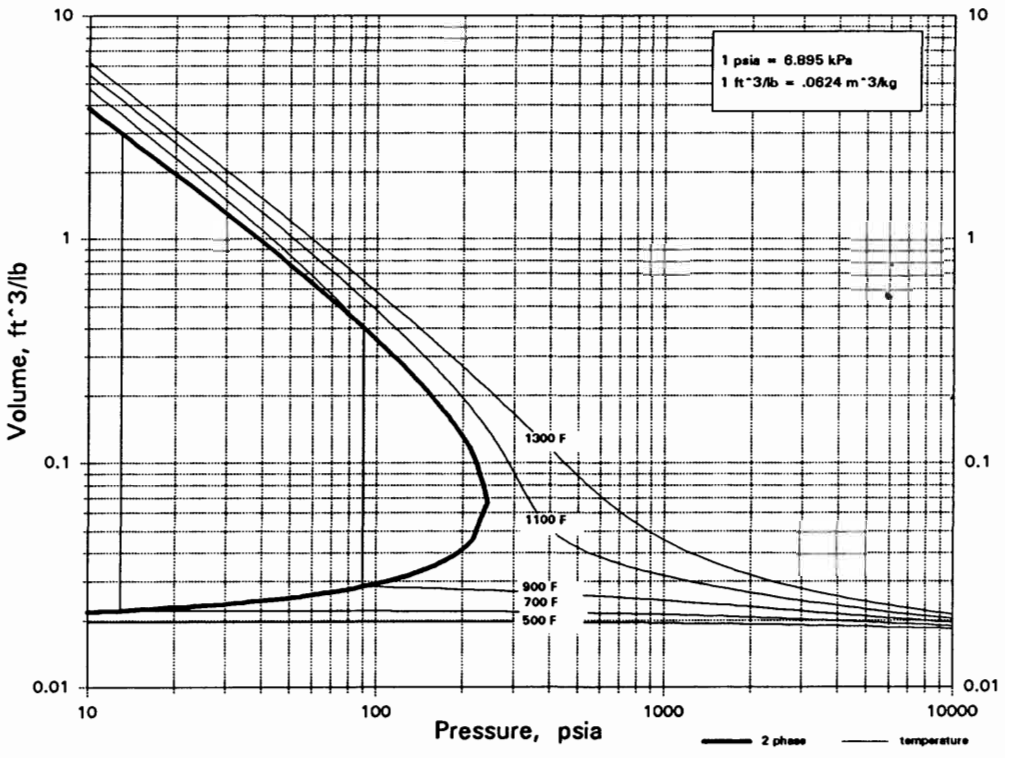


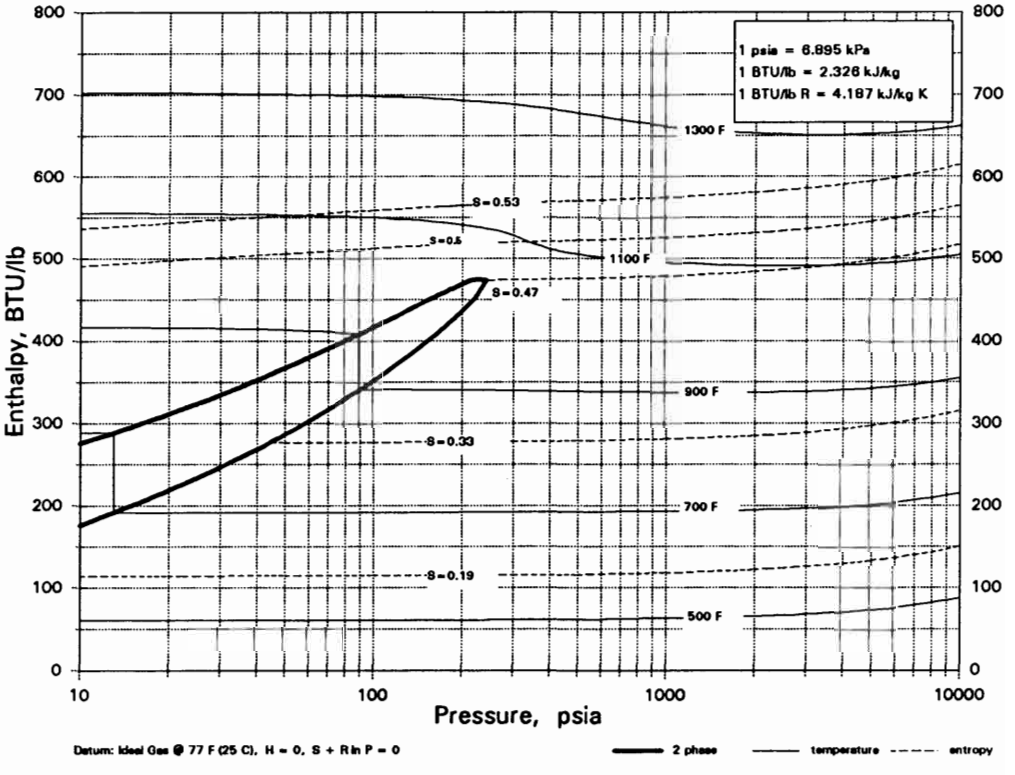
C20H28 1-n-DECYLNAPHTHALENE



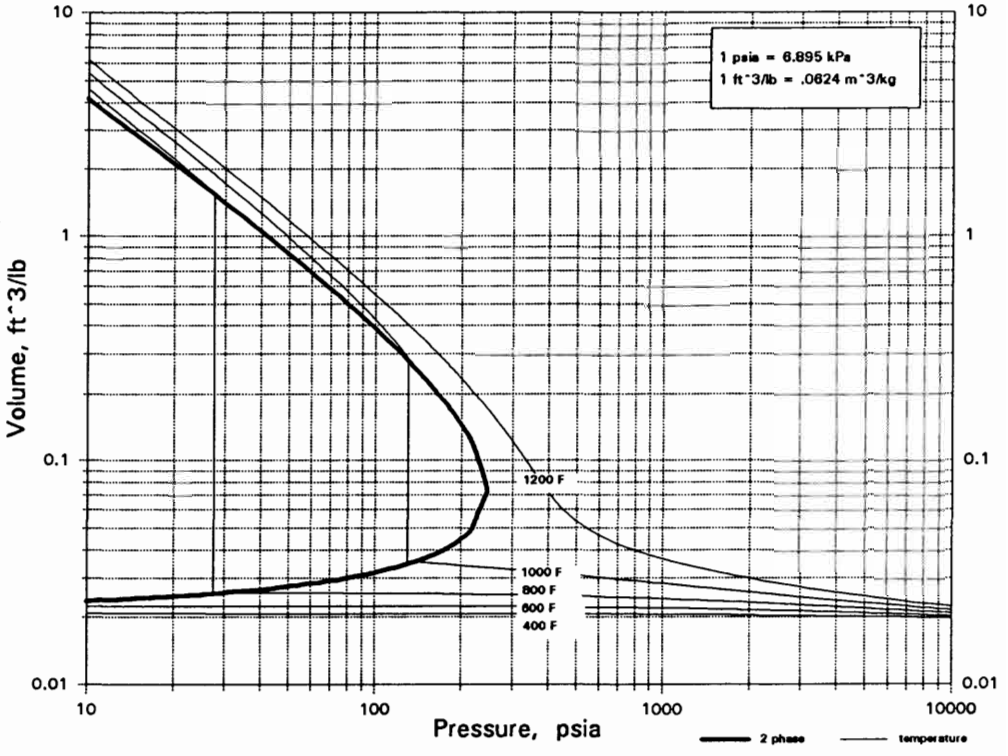


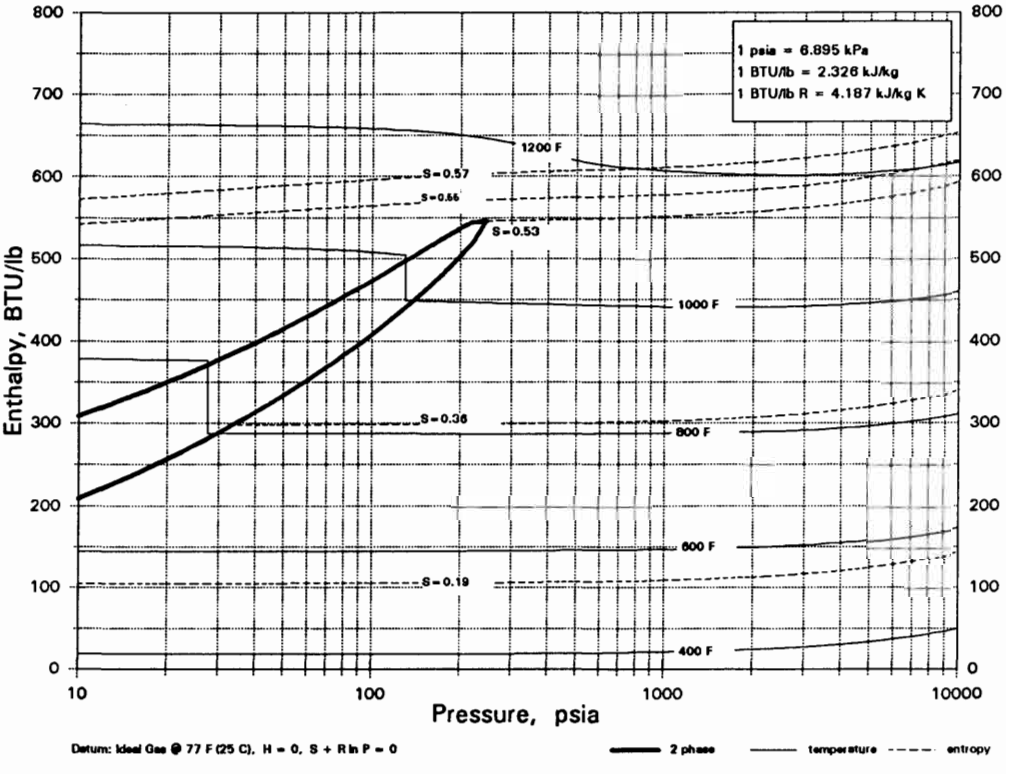
C20H30O2 ABIETIC ACID



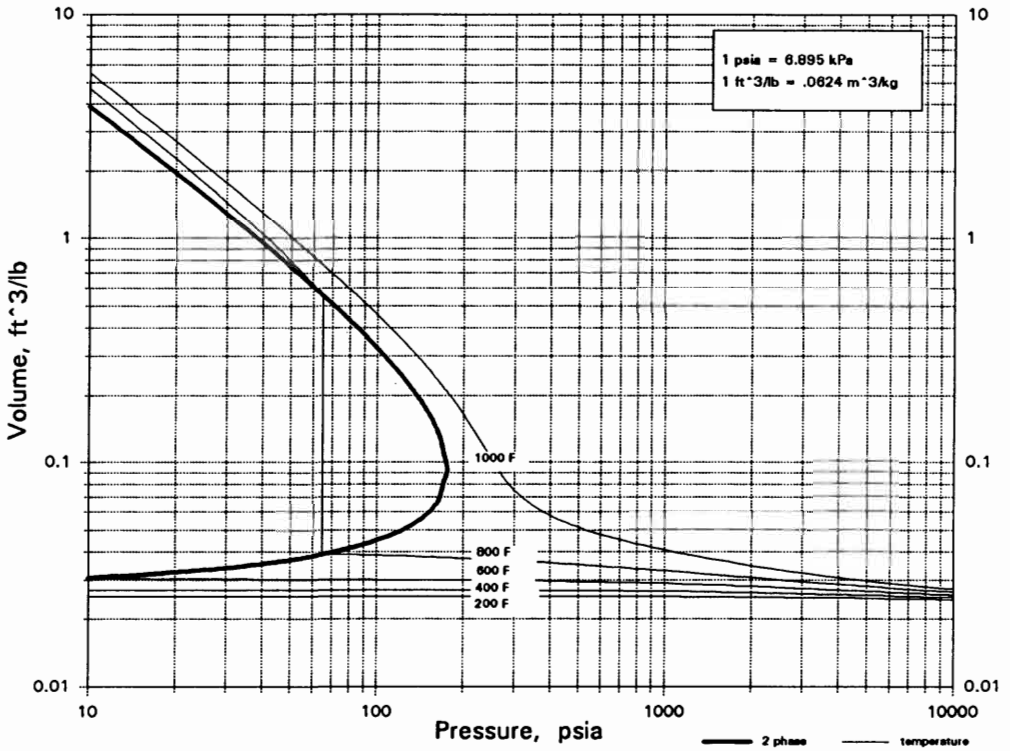


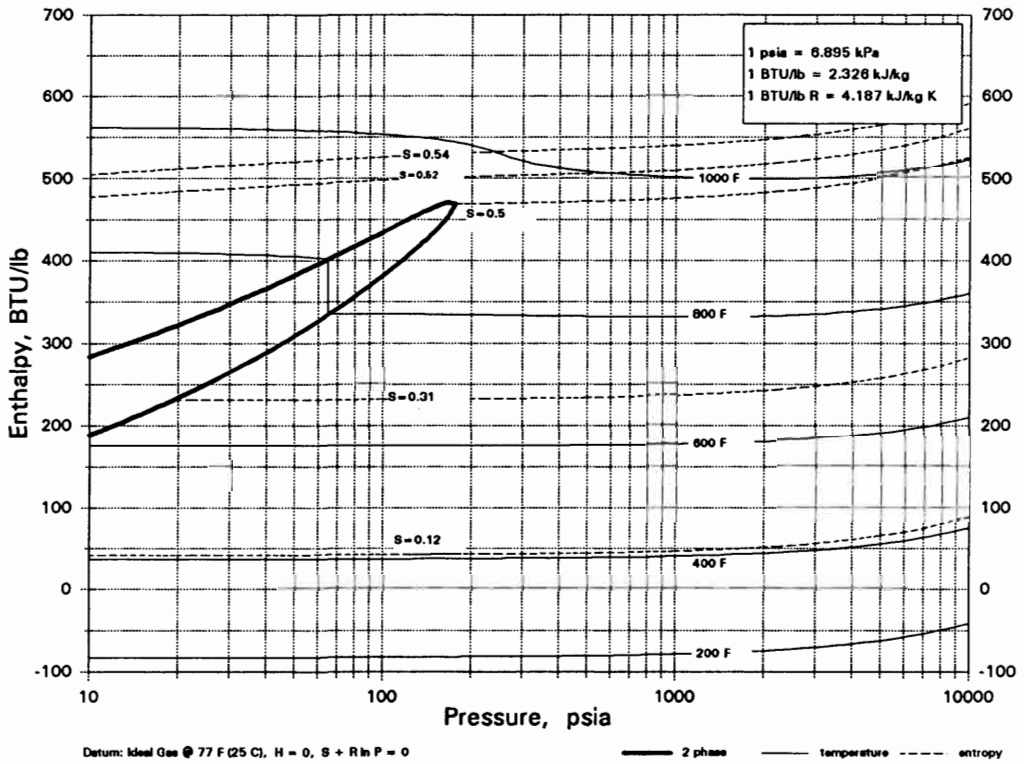
C20H31N DEHYDROABIETYLAMINE



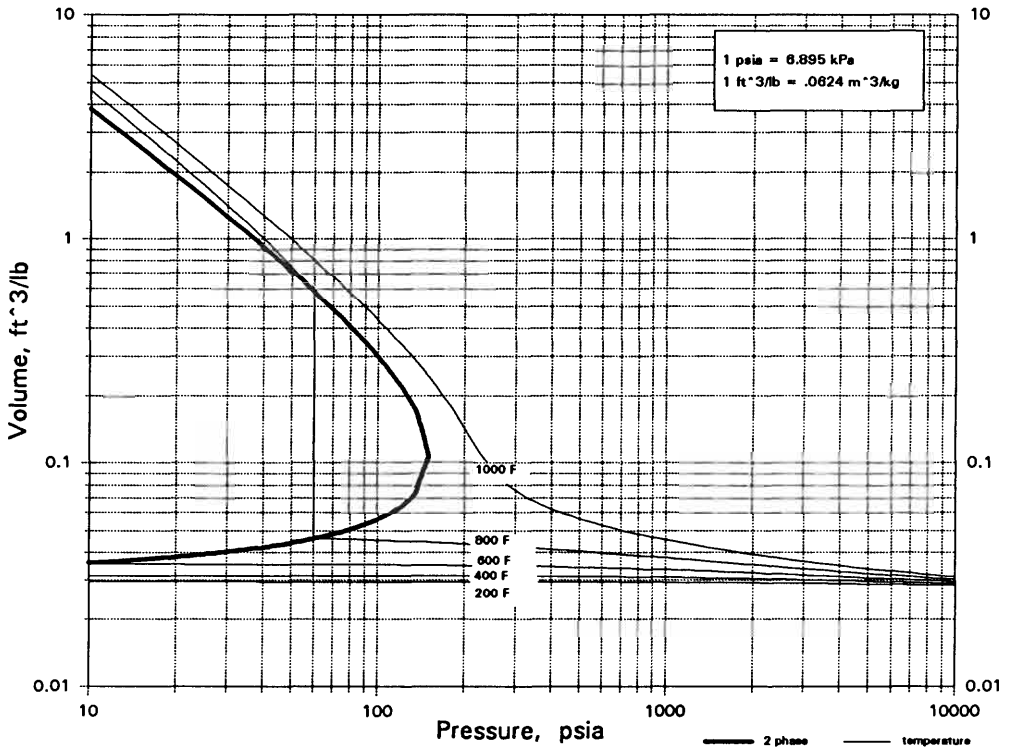


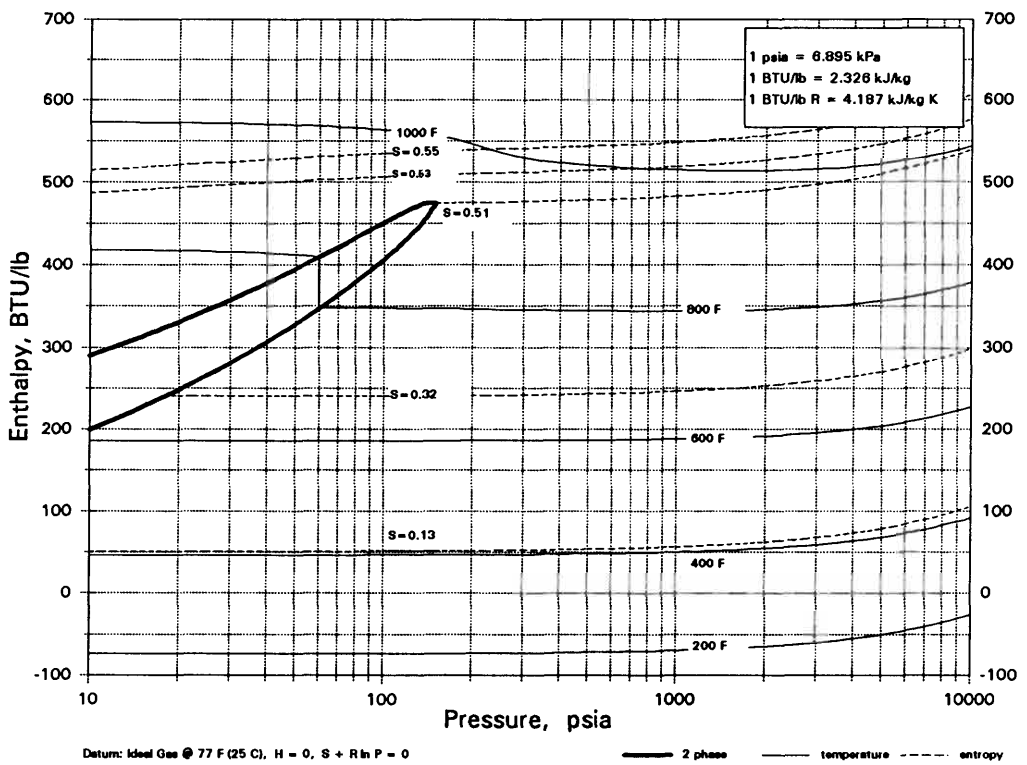
C20H40 1-EICOSENE



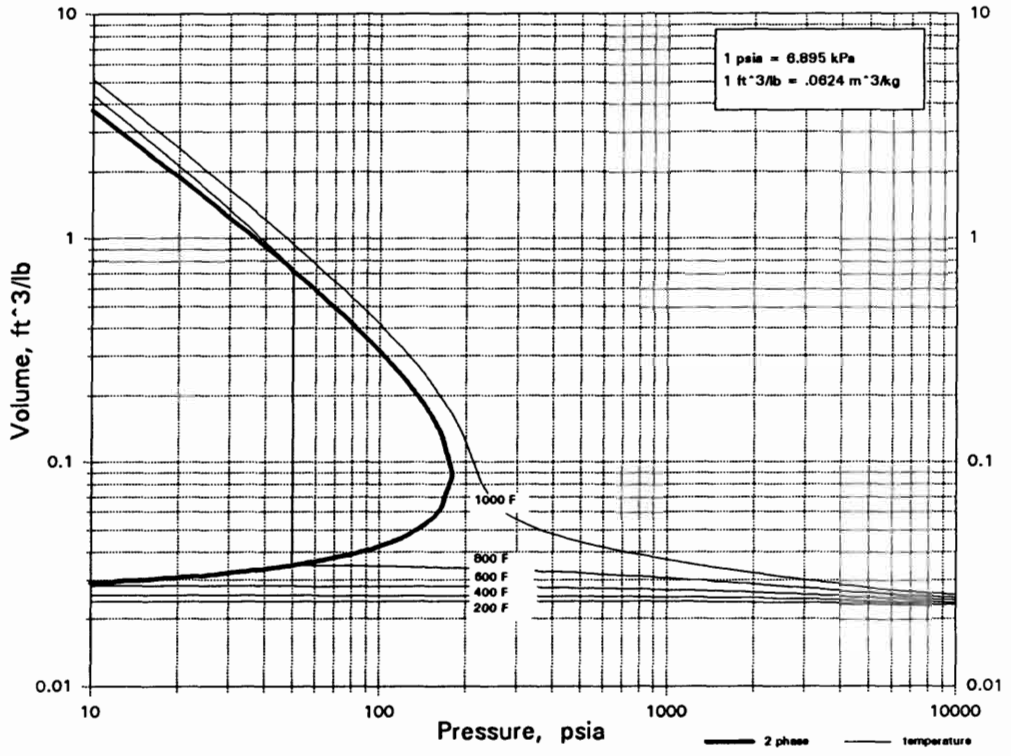


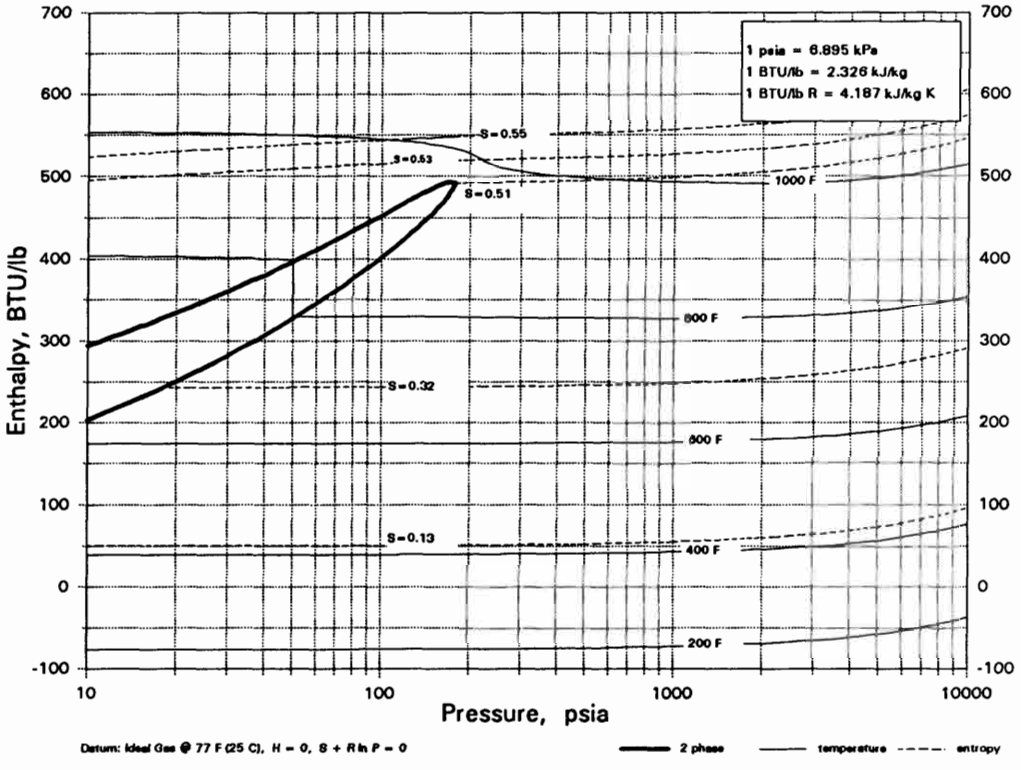
C20H42 n-EICOSANE





C20H42O 1-EICOSANOL





C21H21O4P TRI-o-CRESYL PHOSPHATE

1. Molecular Weight, lb/mol..... 368.37

2. Boiling Point, K..... ----

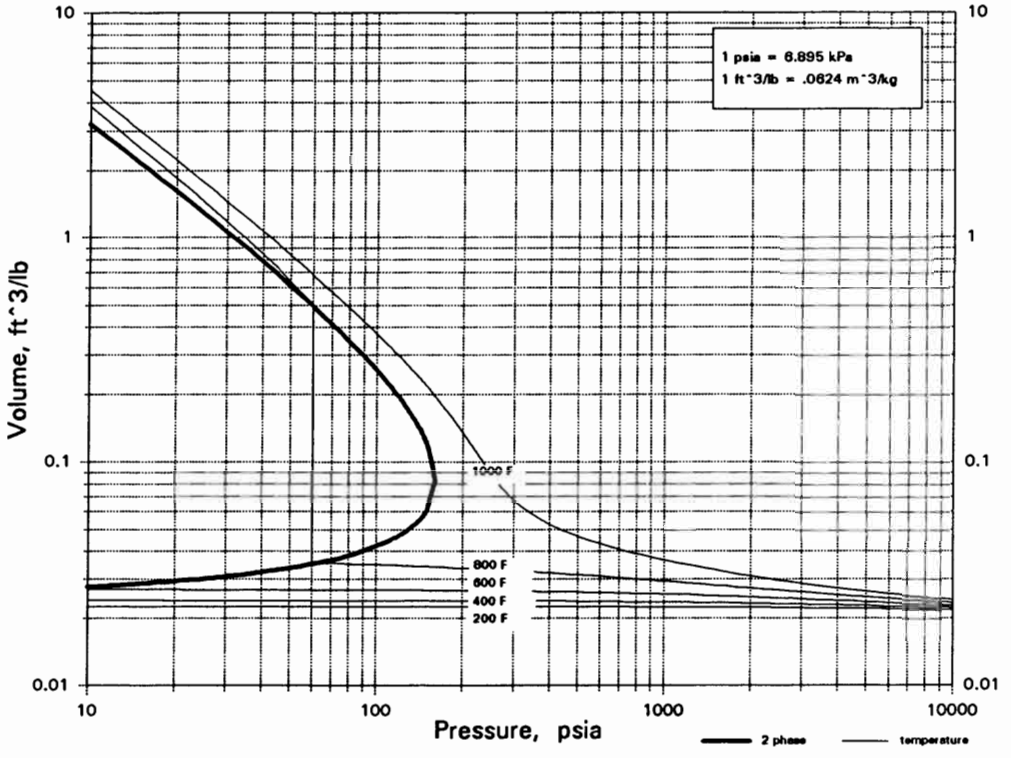
Critical data (Tc, Pc) are not available.

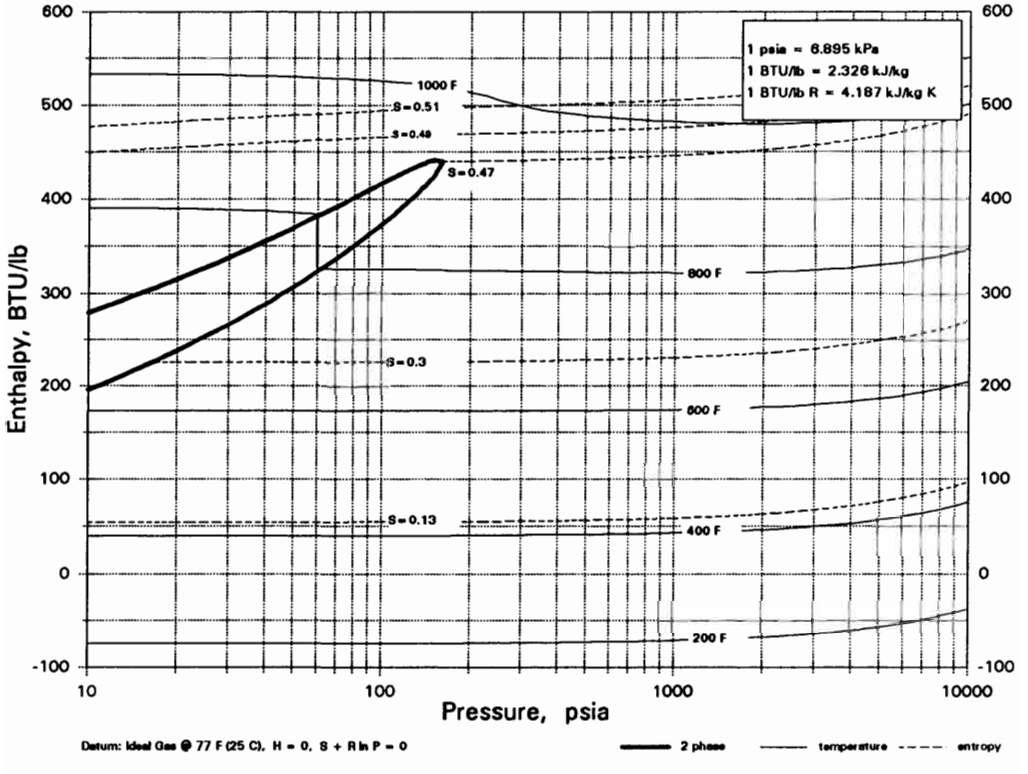
1. Molecular Weight, lb/mol..... 368.37

2. Boiling Point, K..... ----

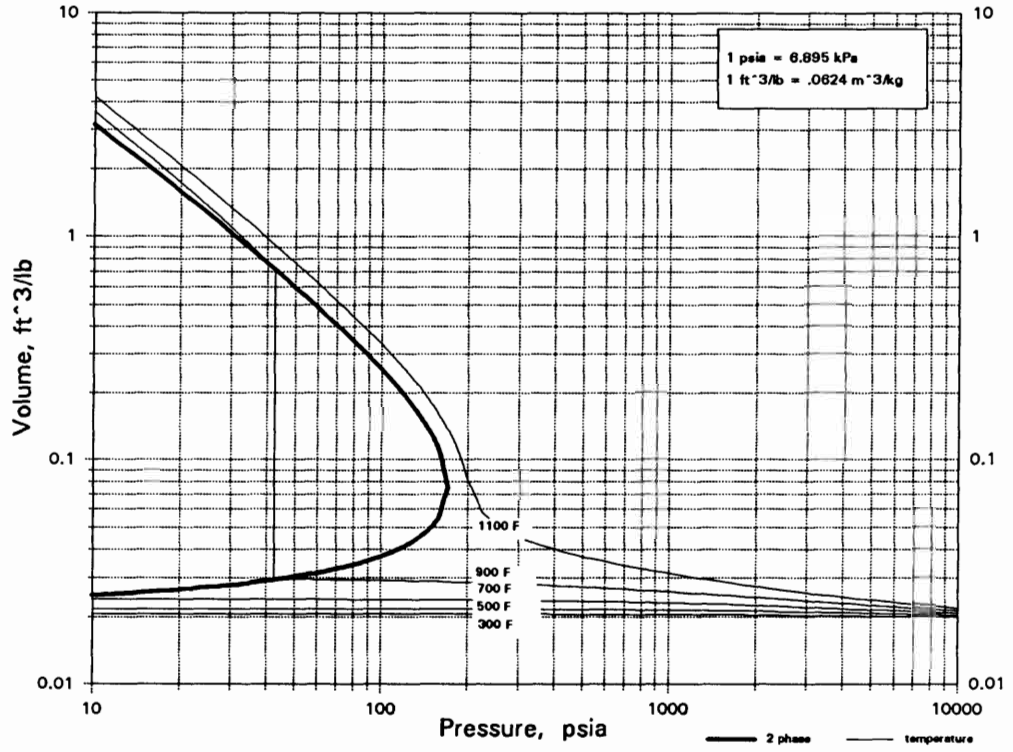
Critical data (Tc, Pc) are not available.

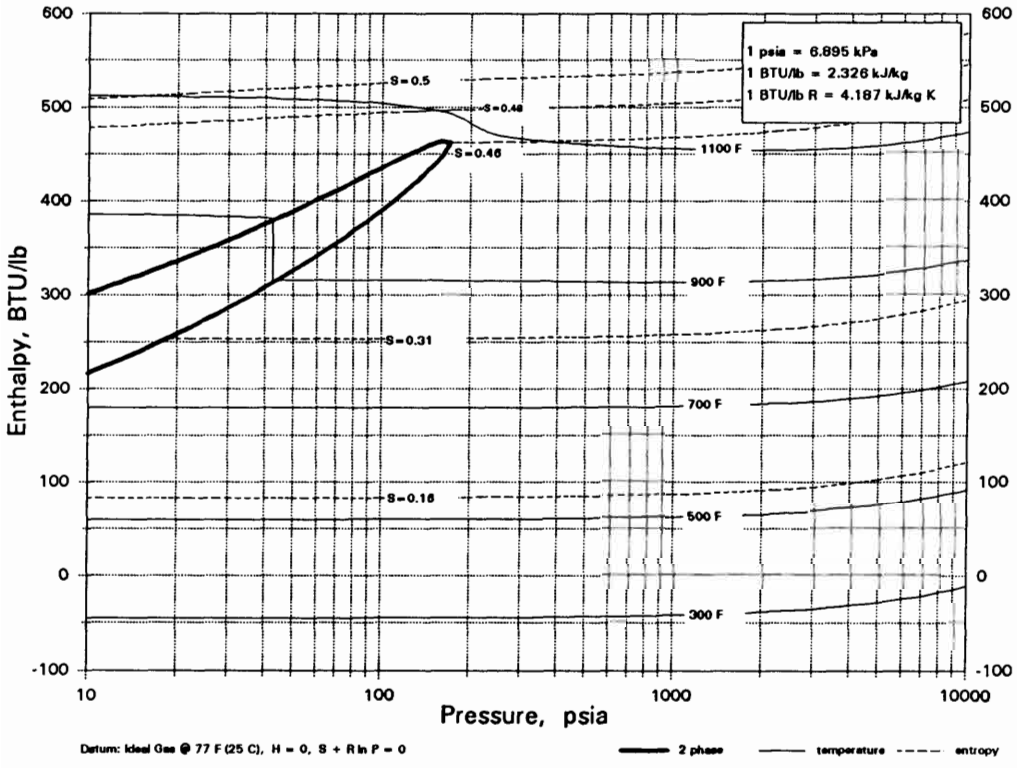
C22H44O2 n-BUTYL STEARATE





C24H38O4 DIISOOCTYL PHTHALATE





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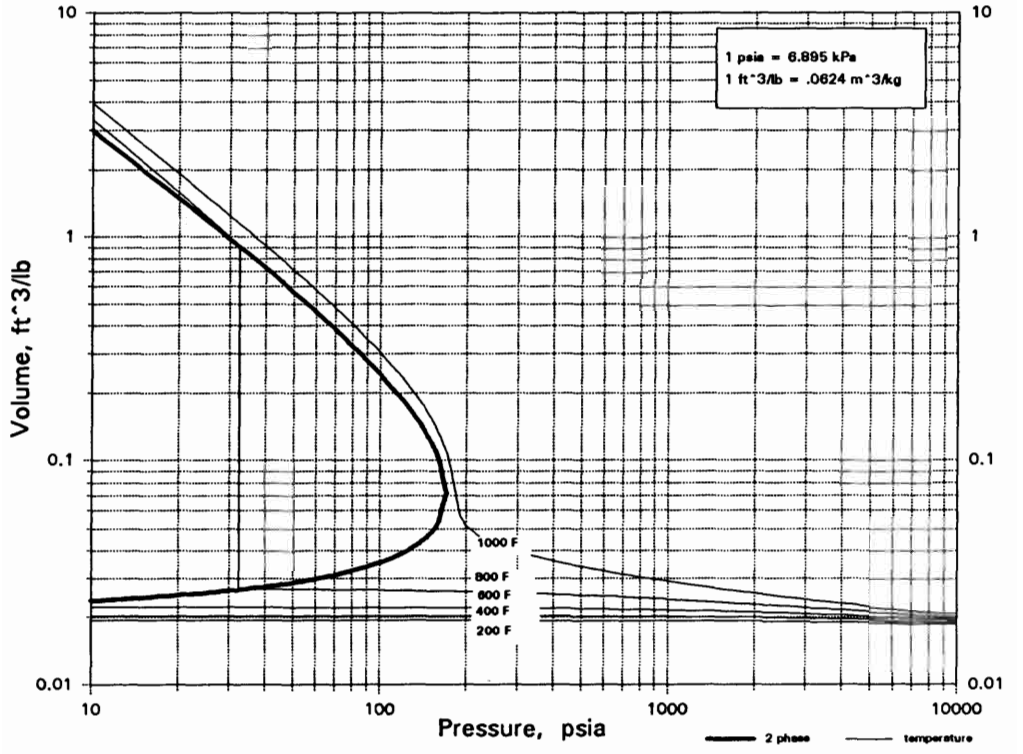
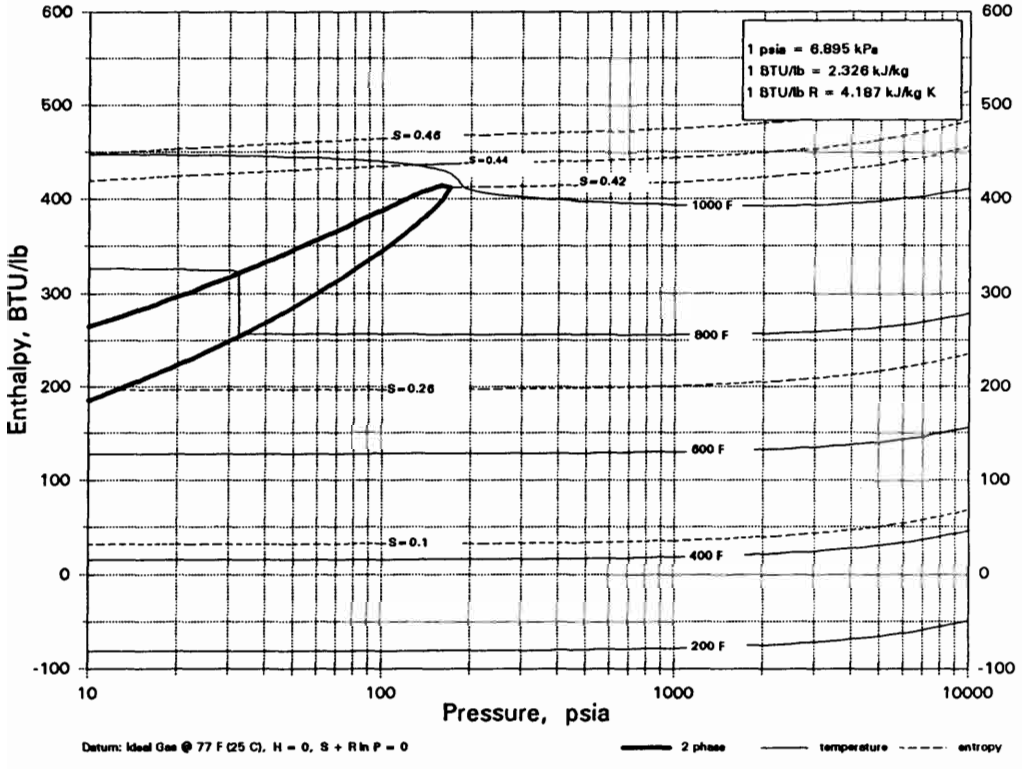
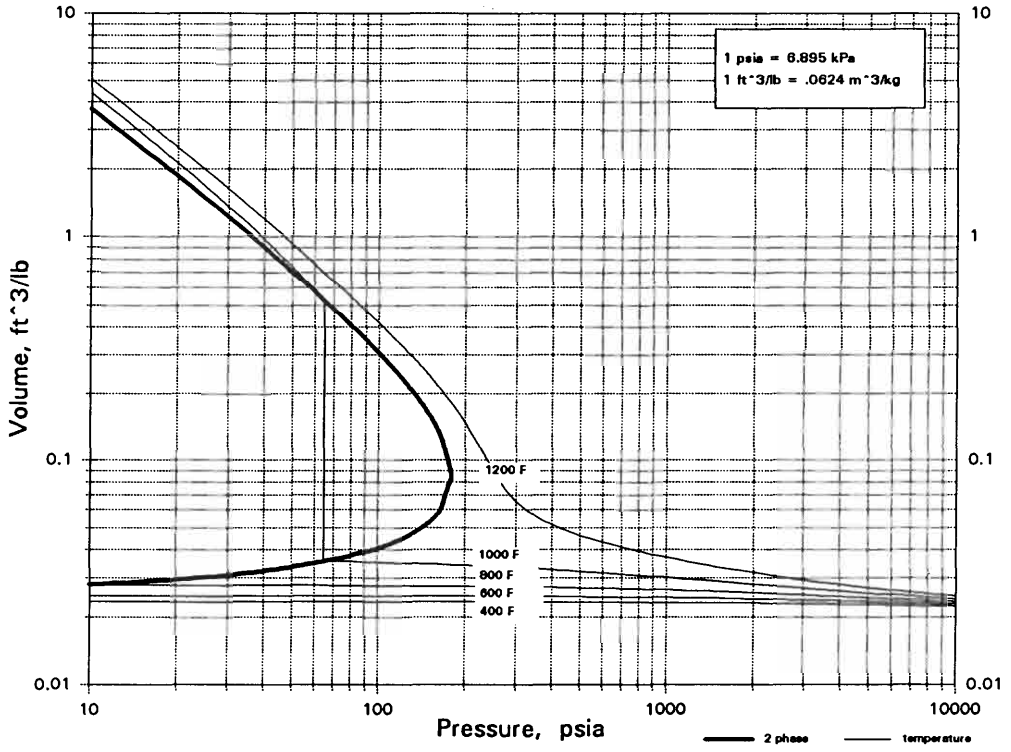
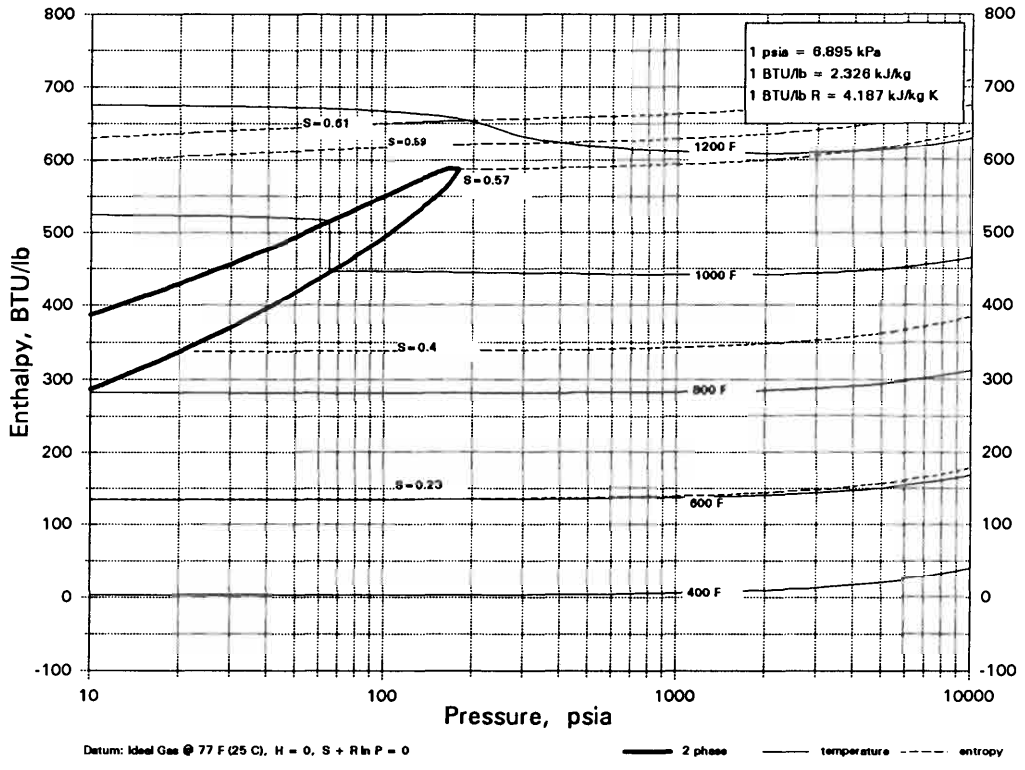


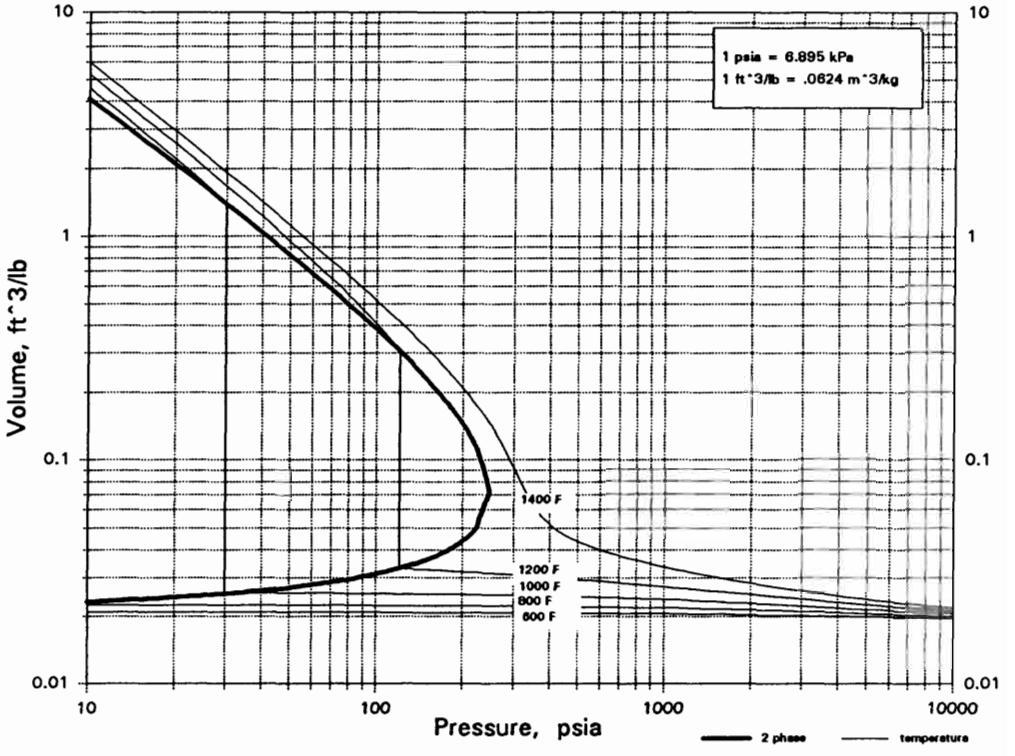


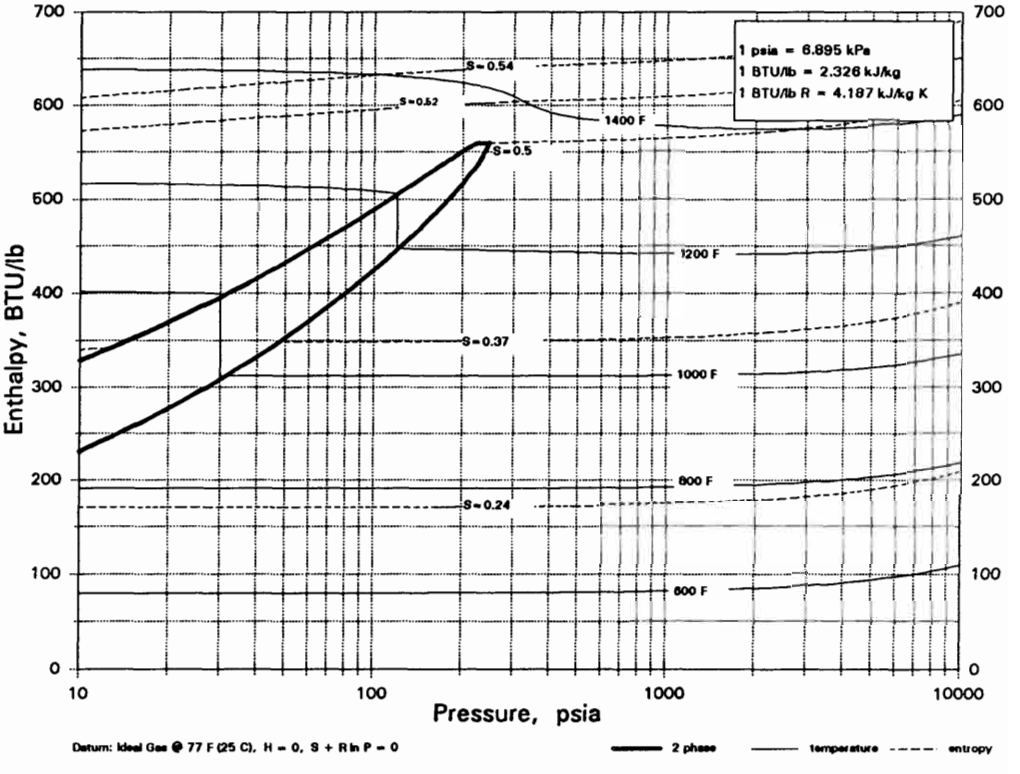
C24H42O DINONYLPHENOL



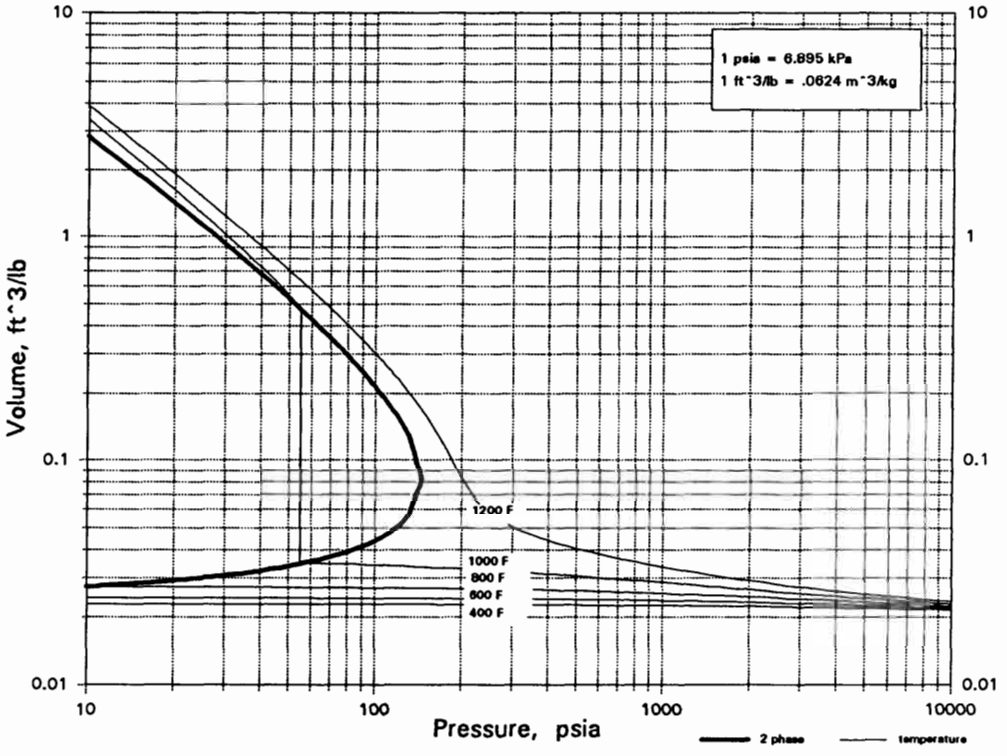


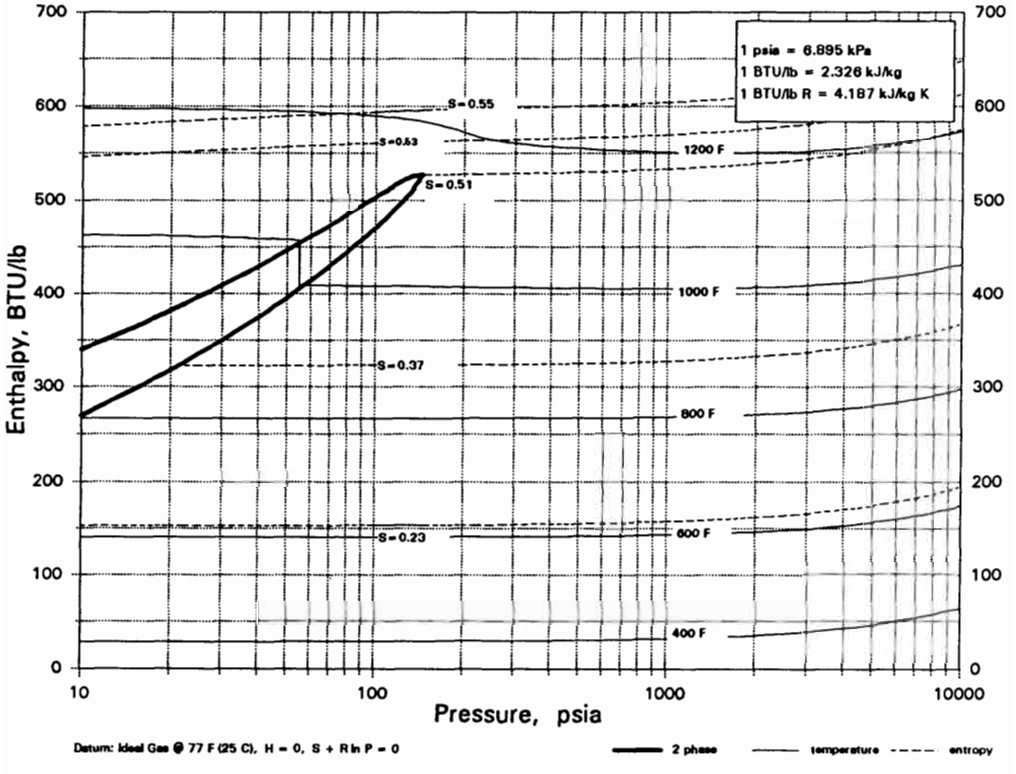
C26H20 TETRAPHENYLETHYLENE





C28H46O4 DIISODECYL PHTHALATE





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Appendix A

Equations for Thermodynamic Properties

Enthalpy

$$H = H_{ref} + \int_{T_{ref}}^{T} C_p \, dT - \Delta H^{resid} \tag{1}$$

Entropy

$$S = S_{ref} + \int_{T_{ref}}^{T} \frac{C_p}{T} \, dT - R \ln\left(\frac{P}{P_{ref}}\right) - \Delta S^{resid} \tag{2}$$

Internal Energy

$$U = H - P\,V \tag{3}$$

Helmholtz Energy

$$A = U - T\,S \tag{4}$$

Gibbs Energy

$$G = H - T\,S \tag{5}$$

Parameters

$$C_p = \text{heat capacity of ideal gas} \tag{6}$$

$$H_{ref}\ ,\ S_{ref} = \text{reference state for ideal gas} \tag{7}$$

$$T_{ref}\ , P_{ref} = \text{reference temperature , reference pressure} \tag{8}$$

$$\Delta H^{resid}\ ,\ \Delta S^{resid} = \text{residual enthalpy , residual entropy} \tag{9}$$

Appendix B

Peng-Robinson Equation of State for Thermodynamic Properties

Equation of State

$$P = \frac{RT}{V - b} - \frac{a}{V(V + b) + b(V - b)} \tag{1}$$

Volume

$$V^3 + (b - \frac{RT}{P})V^2 + (\frac{a}{P} - 3b^2 - \frac{RT}{P}2b)V + (b^3 + \frac{RT}{P}b^2 - \frac{ab}{P}) = 0 \tag{2}$$

Compressibility Factor

$$Z^3 - (1 - B)Z^2 + (A - 3B^2 - 2B)Z - (AB - B^2 - B^3) = 0 \tag{3}$$

Fugacity Coefficient

$$\ln \phi = Z - 1 - \ln(Z - B) - \frac{A}{2\sqrt{2}B}\ln\left(\frac{Z + 2.414B}{Z - 0.414B}\right) \tag{4}$$

Residual Enthalpy

$$\frac{\Delta H^{resid}}{RT} = 1 - Z + \frac{A}{2\sqrt{2}B}(1 + \frac{D}{a})\ln\left(\frac{Z + 2.414B}{Z - 0.414B}\right) \tag{5}$$

Residual Entropy

$$\frac{\Delta S^{resid}}{R} = -\ln(Z - B) + \frac{AD}{2\sqrt{2}Ba}\ln\left(\frac{Z + 2.414B}{Z - 0.414B}\right) \tag{6}$$

Parameters

$$a = a_c\alpha \tag{7}$$

$$a_c = 0.45724R^2T_c^2/P_c \tag{8}$$

$$b = 0.07780RT_c/P_c \tag{9}$$

$$\alpha = [1 + m(1 - T_r^{1/2})]^2 \tag{10}$$

$$m = 0.37464 + 1.54226\Omega - 0.26992\Omega^2 \ (original\ PR) \tag{11}$$

$$m = see\ Stryjek\ ,\ Vera\ (modified\ PR) \tag{12}$$

$$A = aP/R^2T^2 = 0.45724\alpha P_r/T_r^2 = 0.45724\frac{(P/P_c)}{(T/T_c)^2}\alpha \tag{13}$$

$$B = bP/RT = 0.07780P_r/T_r = 0.07780\frac{(P/P_c)}{(T/T_c)} \tag{14}$$

$$D = -T\frac{da}{dT} = ma\sqrt{T_r/\alpha} \tag{15}$$

Appendix C

Examples for Thermodynamic Diagrams

Example 1 - Vessel Pressure

A vessel containing gaseous 1-octene (C8H16) at 230 psia and 500 F is exposed to a fire in the process area. The temperature in the vessel is 900 F when the fire is extinguished. Estimate the final pressure in the vessel.

Since the vessel size does not change appreciably, this situation maybe approximated by a constant volume process. Using the thermodynamic diagram, the initial volume is about 0.24 ft^3/lb. At this same volume and final temperature, the pressure is:

P_{final} = 460 psia

Example 2 - Reactor Size

A batch reactor is to contain 2,000 lb of 1-octene (C8H16) at 200 psia and 500 F. Estimate the reactor size.

Using the thermodynamic diagram, the volume is about 0.32 ft^3/lb at these conditions. Substitution of this into the equation below for the reactor size provides:

Reactor Size = (2,000 lb) (0.32 ft^3/lb) = 640 ft^3

Example 3 - Process Vessel Size

A process vessel is to contain 500 lb of 1-octene (C8H16) at 100 psia and 500 F. Estimate the process vessel size.

Using the thermodynamic diagram, the volume is about 0.8 ft^3/lb at these conditions. Substitution of this into the equation below for the process vessel size provides:

Vessel Size = (500 lb) (0.8 ft^3/lb) = 400 ft^3

Example 4 - Heat Exchanger Duty

1-Octene (C8H16, 30,000 lb/hr) at 100 psia and 500 F is heated to 900 F and then fed to a plug-flow reactor. Estimate the heat exchanger duty necessary to accomplish the heating.

Substitution of mass flow and enthalpies from the thermodynamic diagram into the equation below provides:

Heat Exchanger Duty = mass flow (H_2 - H_1) = (30,000 lb/hr)(475 - 200) BTU/lb

= 8.25 million BTU/hr

Example 5 - Compression

1-Octene (C8H16, 20,000 lb/hr) at 10 psia and 500 F is compressed to 4,000 psia. Estimate the change in enthalpy for the compression assuming adibatic and reversible conditions (constant entropy).

Substitution of mass flow and enthalpies from the thermodynamic diagram into the equation below provides:

Enthalpy Change = mass flow (H_2 - H_1) = (20,000 lb/hr)(310 - 210) BTU/lb

= 2.0 million BTU/hr

This change in enthalpy represents energy that is required to accomplish the compression under adibatic and reversible conditions. Under operating conditions, the actual energy that is required for the compression will be somewhat more depending on the efficiency.

Example 6 - Expansion

1-Octene (C8H16, 30,000 lb/hr) at 8,000 psia and 900 F is expanded to 10 psia. Estimate the change in enthalpy for the expansion assuming adibatic and reversible conditions (constant entropy).

Substitution of mass flow and enthalpies from the thermodynamic diagram into the equation below provides:

Enthalpy Change = mass flow (H_2 - H_1) = (30,000 lb/hr)(280 - 420) BTU/lb

= - 4.2 million BTU/hr

This change in enthalpy represents energy that is available from the expansion under adibatic and reversible conditions. Under operating conditions, the actual energy that is available for the expansion will be somewhat less depending on the efficiency.

Appendix D

CRITICAL CONSTANTS AND ACENTRIC FACTOR FOR C_8 TO C_{28} COMPOUNDS

Carl L. Yaws
Lamar University, Beaumont, Texas

NO	FORMULA	NAME	MW g/mol	T_F K	T_B K	T_C K	P_C bar	V_C cm^3/mol	ρ_C g/cm^3	Z_C	ω
1	C8H4Cl2O2	ISOPHTHALOYL CHLORIDE	203.024	317.00	549.00	768.00	33.30	471.0	0.4310	0.246	0.646
2	C8H4O3	PHTHALIC ANHYDRIDE	148.118	404.26	557.65	791.00	47.20	421.0	0.3518	0.302	0.708
3	C8H6O4	ISOPHTHALIC ACID	166.133	619.15	753.00	1007.00	39.50	424.0	0.3918	0.200	1.062
4	C8H6O4	PHTHALIC ACID	166.133	464.15	598.00	800.00	39.50	424.0	0.3918	0.252	1.059
5	C8H6O4	TEREPHTHALIC ACID	166.133	700.15	832.00	1113.00	39.50	424.0	0.3918	0.181	1.059
6	C8H6S	BENZOTHIOPHENE	134.202	304.50	493.05	754.00	41.40	349.0	0.3845	0.230	0.296
7	C8H7N	INDOLE	117.150	273.68	526.15	790.00	43.00	431.0	0.2718	0.282	0.374
8	C8H8	STYRENE	104.152	242.54	418.31	648.00	40.00	352.0	0.2959	0.261	0.236
9	C8H8O	ACETOPHENONE	120.151	293.65	475.15	701.00	38.40	376.0	0.3196	0.248	0.429
10	C8H8O	p-TOLUALDEHYDE	120.151	---	477.15	698.00	36.70	416.0	0.2888	0.263	0.442
11	C8H8O2	METHYL BENZOATE	136.150	260.75	472.65	693.00	35.90	436.0	0.3123	0.272	0.415
12	C8H8O2	o-TOLUIC ACID	136.150	376.85	532.00	751.00	38.60	397.0	0.3429	0.245	0.657
13	C8H8O2	p-TOLUIC ACID	136.150	452.75	548.15	773.00	38.60	397.0	0.3429	0.238	0.661
14	C8H8O3	METHYL SALICYLATE	152.150	265.15	493.65	701.00	40.90	410.0	0.3711	0.288	0.632
15	C8H8O3	VANILLIN	152.150	355.00	558.00	777.00	40.10	415.0	0.3666	0.258	0.757
16	C8H9NO	ACETANILIDE	135.166	386.65	576.95	825.00	37.30	430.0	0.3143	0.234	0.564
17	C8H10	ETHYLBENZENE	106.167	178.20	409.35	617.17	36.09	373.8	0.2840	0.263	0.304
18	C8H10	m-XYLENE	106.167	225.30	412.27	617.05	35.41	375.8	0.2825	0.259	0.326
19	C8H10	o-XYLENE	106.167	247.98	417.58	630.37	37.34	369.2	0.2876	0.263	0.313
20	C8H10	p-XYLENE	106.167	286.41	411.51	616.26	35.11	379.1	0.2801	0.260	0.326
21	C8H10O	m-ETHYLPHENOL	122.167	---	477.66	716.45	42.90	387.0	0.3157	0.279	0.524
22	C8H10O	p-ETHYLPHENOL	122.167	318.23	491.14	716.45	42.90	387.0	0.3157	0.279	0.524
23	C8H10O	PHENETOLE	122.167	243.63	443.15	647.15	34.25	390.0	0.3132	0.248	0.415
24	C8H10O	2-PHENYLETHANOL	122.167	247.00	492.05	684.00	39.20	387.0	0.3157	0.267	0.743
25	C8H10O	2-3-XYLENOL	122.167	345.71	490.07	722.95	49.00	360.0	0.3394	0.293	0.511
26	C8H10O	2-4-XYLENOL	122.167	297.68	484.13	707.65	44.00	390.0	0.3132	0.292	0.513
27	C8H10O	2-5-XYLENOL	122.167	347.99	484.33	707.05	49.00	350.0	0.3490	0.292	0.563
28	C8H10O	2-6-XYLENOL	122.167	318.76	474.22	701.05	43.00	390.0	0.3132	0.288	0.455
29	C8H10O	3-4-XYLENOL	122.167	338.25	500.15	729.95	50.00	350.0	0.3490	0.288	0.573
30	C8H10O	3-5-XYLENOL	122.167	336.59	494.89	715.65	36.48	480.0	0.2545	0.294	0.491
31	C8H11N	N-N-DIMETHYLANILINE	121.182	275.60	466.69	687.15	36.27	465.0	0.2606	0.295	0.403
32	C8H11N	o-ETHYLANILINE	121.182	226.55	482.65	704.00	37.40	399.0	0.3037	0.255	0.463
33	C8H11N	2-4-6-TRIMETHYLPYRIDINE	121.182	229.00	444.00	653.00	33.30	417.0	0.2906	0.256	0.376
34	C8H11NO	p-PHENETIDINE	137.181	277.00	528.00	754.00	35.70	446.0	0.3076	0.254	0.553
35	C8H12	1-5-CYCLOOCTADIENE	108.183	203.98	423.27	645.00	39.00	366.0	0.2956	0.266	0.286
36	C8H12	VINYLCYCLOHEXENE	108.183	164.00	401.00	599.00	34.30	379.0	0.2854	0.261	0.329
37	C8H12O4	1-4-CYCLOHEXANEDICARBOXYLIC ACID	172.181	585.65	669.00	889.00	34.20	464.0	0.3711	0.215	1.036
38	C8H12O4	DIETHYL MALEATE	172.181	264.35	498.15	680.00	26.10	508.0	0.3389	0.235	0.666
39	C8H14O2	n-BUTYL METHACRYLATE	142.198	---	434.00	616.00	26.30	481.0	0.2956	0.247	0.466
40	C8H14O3	BUTYRIC ANHYDRIDE	158.197	199.85	468.15	639.00	26.90	501.0	0.3158	0.254	0.659
41	C8H14O4	DIETHYL SUCCINATE	174.197	252.35	489.65	660.00	25.30	522.0	0.3337	0.241	0.737
42	C8H16	1-1-DIMETHYLCYCLOHEXANE	112.215	239.66	392.70	591.15	29.38	450.0	0.2494	0.269	0.233
43	C8H16	cis-1-2-DIMETHYLCYCLOHEXANE	112.215	223.16	402.94	606.15	29.38	460.0	0.2439	0.268	0.232
44	C8H16	trans-1-2-DIMETHYLCYCLOHEXANE	112.215	184.99	396.58	596.15	29.38	460.0	0.2439	0.273	0.238
45	C8H16	cis-1-3-DIMETHYLCYCLOHEXANE	112.215	197.58	393.24	591.15	29.38	450.0	0.2494	0.269	0.237
46	C8H16	trans-1-3-DIMETHYLCYCLOHEXANE	112.215	183.07	397.61	598.00	39.38	460.0	0.2439	0.272	0.234
47	C8H16	cis-1-4-DIMETHYLCYCLOHEXANE	112.215	185.72	397.47	598.15	29.38	460.0	0.2439	0.272	0.231
48	C8H16	trans-1-4-DIMETHYLCYCLOHEXANE	112.215	236.21	392.51	590.15	29.38	450.0	0.2494	0.269	0.237
49	C8H16	ETHYLCYCLOHEXANE	112.215	161.84	404.95	609.15	30.40	450.0	0.2494	0.270	0.246
50	C8H16	2-ETHYL-1-HEXENE	112.215	---	393.15	574.00	30.70	399.0	0.2812	0.257	0.380
51	C8H16	1-METHYL-1-ETHYLCYCLOPENTANE	112.215	129.35	394.67	582.00	30.20	428.0	0.2622	0.267	0.330
52	C8H16	1-OCTENE	112.215	171.45	394.44	566.60	25.50	472.0	0.2377	0.256	0.375
53	C8H16	trans-2-OCTENE	112.215	185.45	398.15	577.00	25.80	484.0	0.2318	0.260	0.338
54	C8H16	trans-3-OCTENE	112.215	163.15	396.45	574.00	25.80	480.0	0.2338	0.260	0.344
55	C8H16	trans-4-OCTENE	112.215	179.37	395.41	573.00	25.80	480.0	0.2338	0.260	0.339
56	C8H16	n-PROPYLCYCLOPENTANE	112.215	155.82	404.11	603.00	30.00	425.0	0.2640	0.254	0.272
57	C8H16	2-4-4-TRIMETHYL-1-PENTENE	112.215	179.70	374.59	553.00	26.30	465.0	0.2413	0.266	0.270
58	C8H16	2-4-4-TRIMETHYL-2-PENTENE	112.215	166.84	378.06	558.00	26.30	470.0	0.2388	0.266	0.265
59	C8H16O	2-ETHYLHEXANAL	128.214	---	433.80	607.00	25.80	474.0	0.2705	0.242	0.520
60	C8H16O	1-OCTANAL	128.214	246.00	447.15	621.00	25.50	474.0	0.2705	0.234	0.547
61	C8H16O	2-OCTANONE	128.214	252.85	445.75	624.00	26.40	469.0	0.2734	0.239	0.528
62	C8H16O2	n-BUTYL n-BUTYRATE	144.214	181.15	438.15	616.00	25.40	494.0	0.2919	0.245	0.485
63	C8H16O2	n-HEXYL ACETATE	144.214	192.25	444.65	618.00	25.40	494.0	0.2919	0.244	0.540
64	C8H16O2	ISOBUTYL ISOBUTYRATE	144.214	192.45	420.65	602.00	26.10	494.0	0.2919	0.258	0.395

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65	C8H16O2	n-OCTANOIC ACID	144.214	289.65	513.05	692.00	26.90	494.0	0.2919	0.231	0.779
66	C8H16O4	DIETHYLENE GLYCOL ETHYL ETHER ACETAT	176.213	248.15	490.55	660.00	24.20	565.0	0.3119	0.249	0.715
67	C8H18	2-2-DIMETHYLHEXANE	114.231	151.97	379.99	549.80	25.30	478.0	0.2390	0.265	0.338
68	C8H18	2-3-DIMETHYLHEXANE	114.231	---	388.76	563.40	26.30	468.2	0.2440	0.263	0.347
69	C8H18	2-4-DIMETHYLHEXANE	114.231	---	382.58	553.50	25.60	472.0	0.2420	0.263	0.344
70	C8H18	2-5-DIMETHYLHEXANE	114.231	182.00	382.26	550.00	24.90	482.0	0.2370	0.262	0.358
71	C8H18	3-3-DIMETHYLHEXANE	114.231	147.05	385.12	562.00	26.50	442.8	0.2580	0.251	0.320
72	C8H18	3-4-DIMETHYLHEXANE	114.231	---	390.88	568.80	26.90	466.2	0.2450	0.265	0.338
73	C8H18	3-ETHYLHEXANE	114.231	---	391.69	565.40	26.10	455.1	0.2510	0.253	0.363
74	C8H18	3-METHYL-3-ETHYLPENTANE	114.231	182.28	391.42	576.50	28.10	455.1	0.2510	0.267	0.305
75	C8H18	2-METHYLHEPTANE	114.231	164.16	390.80	559.64	24.85	488.0	0.2341	0.261	0.377
76	C8H18	3-METHYLHEPTANE	114.231	152.60	392.08	563.67	25.46	464.0	0.2462	0.252	0.372
77	C8H18	4-METHYLHEPTANE	114.231	152.20	390.86	561.74	25.42	476.0	0.2400	0.259	0.371
78	C8H18	n-OCTANE	114.231	216.38	398.83	568.83	24.86	492.1	0.2322	0.259	0.396
79	C8H18	2-2-3-TRIMETHYLPENTANE	114.231	160.89	383.00	563.50	27.30	436.0	0.2620	0.254	0.297
80	C8H18	2-2-4-TRIMETHYLPENTANE	114.231	165.78	372.39	543.96	25.68	468.0	0.2441	0.266	0.303
81	C8H18	2-3-3-TRIMETHYLPENTANE	114.231	172.22	387.92	573.50	28.20	455.1	0.2510	0.269	0.290
82	C8H18	2-3-4-TRIMETHYLPENTANE	114.231	163.95	386.62	566.30	27.30	460.6	0.2480	0.267	0.316
83	C8H18O	DI-n-BUTYL ETHER	130.230	177.95	413.44	581.00	24.60	487.0	0.2674	0.248	0.467
84	C8H18O	DI-sec-BUTYL ETHER	130.230	173.15	394.20	559.00	25.30	494.0	0.2636	0.269	0.432
85	C8H18O	DI-tert-BUTYL ETHER	130.230	195.00	380.40	550.00	25.30	487.0	0.2674	0.269	0.346
86	C8H18O	2-ETHYL-1-HEXANOL	130.230	203.15	457.75	640.25	27.30	485.0	0.2685	0.249	0.549
87	C8H18O	1-OCTANOL	130.230	257.65	468.35	652.50	28.60	490.0	0.2658	0.258	0.594
88	C8H18O	2-OCTANOL	130.230	241.55	452.95	637.15	27.30	469.0	0.2777	0.242	0.506
89	C8H18O2	DI-t-BUTYL PEROXIDE	146.230	233.15	384.15	547.00	24.80	508.0	0.2879	0.277	0.403
90	C8H18O2S	DI-n-BUTYL SULFONE	178.296	318.00	564.00	767.00	25.40	569.0	0.3133	0.227	0.688
91	C8H18O3	DIETHYLENE GLYCOL DIETHYL ETHER	162.229	228.85	462.15	624.00	23.70	558.0	0.2907	0.255	0.681
92	C8H18O3	DIETHYLENE GLYCOL MONOBUTYL EHTER	162.229	205.15	504.15	654.00	25.60	526.0	0.3084	0.248	0.937
93	C8H18O4	TRIETHYLENE GLYCOL DIMETHYL ETHER	178.229	229.35	489.15	651.00	23.10	548.0	0.3252	0.234	0.792
94	C8H18O5	TETRAETHYLENE GLYCOL	194.228	268.15	581.00	722.00	25.90	564.0	0.3444	0.243	1.578
95	C8H18S	n-OCTYL MERCAPTAN	146.297	223.95	472.19	664.00	25.20	518.0	0.2824	0.236	0.473
96	C8H18S	tert-OCTYL MERCAPTAN	146.297	199.00	429.00	627.00	25.90	529.0	0.2766	0.263	0.307
97	C8H19N	DI-n-BUTYLAMINE	129.246	211.15	432.00	607.50	31.10	524.0	0.2467	0.323	0.560
98	C8H19N	DIISOBUTYLAMINE	129.246	203.15	412.25	580.00	25.70	524.0	0.2467	0.279	0.485
99	C8H19N	n-OCTYLAMINE	129.246	272.75	452.75	627.00	25.80	524.0	0.2467	0.259	0.568
100	C8H23N5	TETRAETHYLENEPENTAMINE	189.304	243.00	606.15	774.00	25.30	636.0	0.2976	0.250	1.237
101	C8H24O4Si4	OCTAMETHYLCYCLOTETRASILOXANE	296.618	290.80	448.15	586.50	13.32	970.0	0.3058	0.265	0.589
102	C9H4O5	TRIMELLITIC ANHYDRIDE	192.128	438.15	663.00	890.00	40.80	462.0	0.4159	0.255	1.050
103	C9H6N2O2	TOLUENE DIISOCYANATE	174.159	287.04	523.15	737.00	30.40	525.0	0.3317	0.260	0.553
104	C9H7N	ISOQUINOLINE	129.161	299.45	516.40	803.15	49.80	403.0	0.3205	0.301	0.289
105	C9H7N	QUINOLINE	129.161	258.25	510.75	782.15	46.60	469.0	0.2754	0.336	0.329
106	C9H7NO	8-HYDROXYQUINOLINE	145.161	346.00	540.00	788.00	43.60	414.0	0.3506	0.276	0.522
107	C9H8	INDENE	116.163	271.70	455.77	687.00	38.20	368.0	0.3157	0.246	0.335
108	C9H8O	2-METHYLBENZOFURAN	132.162	---	470.65	698.00	36.40	405.0	0.3263	0.254	0.374
109	C9H10	INDANE	118.178	221.74	451.12	684.90	39.50	381.0	0.3102	0.264	0.309
110	C9H10	alpha-METHYLSTYRENE	118.178	249.95	438.65	654.00	33.60	423.0	0.2794	0.261	0.327
111	C9H10	m-METHYLSTYRENE	118.178	186.81	444.75	657.00	32.90	407.0	0.2904	0.245	0.349
112	C9H10	o-METHYLSTYRENE	118.178	204.58	442.96	659.00	34.70	407.0	0.2904	0.258	0.341
113	C9H10	p-METHYLSTYRENE	118.178	239.02	445.93	665.00	33.60	431.0	0.2742	0.262	0.318
114	C9H10O2	BENZYL ACETATE	150.177	221.65	486.65	699.00	31.80	449.0	0.3345	0.246	0.470
115	C9H10O2	ETHYL BENZOATE	150.177	238.45	486.55	698.00	31.80	489.0	0.3071	0.268	0.479
116	C9H10O3	ETHYL VANILLIN	166.177	350.65	567.00	748.00	32.70	467.0	0.3558	0.246	1.073
117	C9H11NO	p-DIMETHYLAMINOBENZALDEHYDE	149.192	348.00	588.00	832.00	30.70	471.0	0.3168	0.209	0.527
118	C9H12	CUMENE	120.194	177.14	425.56	631.15	32.09	427.7	0.2810	0.262	0.338
119	C9H12	m-ETHYLTOLUENE	120.194	177.61	434.48	637.15	28.37	490.0	0.2453	0.262	0.322
120	C9H12	o-ETHYLTOLUENE	120.194	192.35	438.33	651.15	30.40	460.0	0.2613	0.258	0.293
121	C9H12	p-ETHYLTOLUENE	120.194	210.83	435.16	640.15	29.38	470.0	0.2557	0.259	0.324
122	C9H12	MESITYLENE	120.194	228.46	437.89	637.36	31.27	433.0	0.2776	0.256	0.398
123	C9H12	n-PROPYLBENZENE	120.194	173.67	432.39	638.38	32.00	440.0	0.2732	0.265	0.346
124	C9H12	1-2-3-TRIMETHYLBENZENE	120.194	247.79	449.27	664.53	34.54	414.0	0.2903	0.259	0.366
125	C9H12	1-2-4-TRIMETHYLBENZENE	120.194	229.38	442.53	649.13	32.32	430.0	0.2795	0.258	0.379
126	C9H12O	BENZYL ETHYL ETHER	136.194	275.65	458.15	662.00	31.10	442.0	0.3081	0.250	0.433
127	C9H12O	2-PHENYL-2-PROPANOL	136.194	309.15	475.15	660.00	34.90	440.0	0.3095	0.280	0.698
128	C9H12O2	CUMENE HYDROPEROXIDE	152.193	264.26	442.70	605.00	33.40	419.0	0.3632	0.278	0.995
129	C9H14O	ISOPHORONE	138.210	265.05	488.35	715.00	33.30	456.0	0.3031	0.255	0.400
130	C9H14O6	GLYCERYL TRIACETATE	218.207	277.25	532.15	704.00	23.10	625.0	0.3491	0.247	0.839
131	C9H16O4	AZELAIC ACID	188.224	379.65	633.36	811.00	25.60	610.0	0.3086	0.232	1.172
132	C9H18	ISOPROPYLCYCLOHEXANE	126.242	183.76	427.91	627.00	28.50	464.0	0.2721	0.254	0.330
133	C9H18	1-NONENE	126.242	191.78	420.02	593.25	23.30	528.0	0.2391	0.249	0.417
134	C9H18	n-PROPYLCYCLOHEXANE	126.242	178.28	429.90	639.15	28.07	477.0	0.2647	0.252	0.260
135	C9H18O	DIISOBUTYL KETONE	142.241	227.17	441.41	615.00	24.80	522.0	0.2725	0.253	0.512
136	C9H18O	1-NONANAL	142.241	255.15	468.15	640.00	23.30	527.0	0.2699	0.231	0.592
137	C9H18O2	n-BUTYL VALERATE	158.241	180.35	459.65	629.00	23.30	547.0	0.2893	0.244	0.596
138	C9H18O2	n-NONANOIC ACID	158.241	285.55	528.75	703.00	24.50	547.0	0.2893	0.229	0.831
139	C9H18O2	n-OCTYL FORMATE	158.241	234.05	471.95	645.00	23.30	547.0	0.2893	0.238	0.587

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140	C9H20	3-3-DIETHYLPENTANE	128.258	240.12	419.34	610.05	26.75	473.0	0.2712	0.249	0.338
141	C9H20	2-2-DIMETHYL-3-ETHYLPENTANE	128.258	173.68	406.99	590.00	25.70	511.0	0.2510	0.268	0.335
142	C9H20	2-4-DIMETHYL-3-ETHYLPENTANE	128.258	150.79	409.87	591.00	25.30	512.0	0.2505	0.264	0.353
143	C9H20	2-2-DIMETHYLHEPTANE	128.258	160.15	405.84	576.80	23.50	519.0	0.2471	0.254	0.390
144	C9H20	2-6-DIMETHYLHEPTANE	128.258	170.25	408.36	579.00	23.00	520.0	0.2467	0.248	0.393
145	C9H20	3-ETHYLHEPTANE	128.258	158.25	416.35	590.00	23.90	528.0	0.2429	0.257	0.408
146	C9H20	2-METHYLOCTANE	128.258	192.78	416.43	586.75	22.90	541.0	0.2371	0.254	0.422
147	C9H20	3-METHYLOCTANE	128.258	165.55	417.38	590.15	23.41	529.0	0.2425	0.252	0.413
148	C9H20	4-METHYLOCTANE	128.258	159.95	415.59	587.65	23.41	523.0	0.2452	0.251	0.413
149	C9H20	n-NONANE	128.258	219.63	423.97	595.65	23.06	547.7	0.2342	0.255	0.438
150	C9H20	2-2-3-3-TETRAMETHYLPENTANE	128.258	263.26	413.44	610.85	27.36	478.0	0.2683	0.257	0.280
151	C9H20	2-2-3-4-TETRAMETHYLPENTANE	128.258	152.06	406.18	592.15	25.64	490.0	0.2618	0.255	0.311
152	C9H20	2-2-4-4-TETRAMETHYLPENTANE	128.258	206.95	395.44	571.35	23.61	504.0	0.2545	0.250	0.316
153	C9H20	2-2-5-TRIMETHYLHEXANE	128.258	167.39	397.24	568.05	23.31	519.0	0.2471	0.256	0.357
154	C9H20O	2-6-DIMETHYL-4-HEPTANOL	144.257	208.00	451.00	603.00	25.50	538.0	0.2681	0.274	0.802
155	C9H20O	1-NONANOL	144.257	268.15	486.25	673.00	26.00	546.4	0.2640	0.254	0.594
156	C9H20O	2-NONANOL	144.257	238.15	471.65	623.00	24.80	538.0	0.2681	0.258	0.890
157	C9H20S	n-NONYL MERCAPTAN	160.324	253.05	492.95	681.00	23.10	571.0	0.2808	0.233	0.531
158	C9H21N	n-NONYLAMINE	143.272	273.15	475.35	648.00	23.60	577.0	0.2483	0.253	0.615
159	C9H21N	TRIPROPYLAMINE	143.272	179.65	429.65	577.50	22.30	576.0	0.2487	0.268	0.699
160	C10H6O8	PYROMELLITIC ACID	254.153	554.00	722.00	893.00	31.40	584.0	0.4352	0.247	1.830
161	C10H7Br	1-BROMONAPHTHALENE	207.070	279.35	554.25	824.00	37.00	453.0	0.4571	0.245	0.369
162	C10H7Cl	1-CHLORONAPHTHALENE	162.618	269.15	532.45	785.00	34.00	434.0	0.3747	0.226	0.383
163	C10H8	NAPHTHALENE	128.174	353.43	491.14	748.35	40.51	413.0	0.3103	0.269	0.302
164	C10H9N	QUINALDINE	143.188	272.15	519.75	773.00	29.60	490.0	0.2922	0.226	0.280
165	C10H10	m-DIVINYLBENZENE	130.189	206.25	472.65	692.00	31.20	440.0	0.2959	0.239	0.373
166	C10H10	1-METHYLINDENE	130.189	---	471.65	703.00	34.60	440.0	0.2959	0.260	0.336
167	C10H10	2-METHYLINDENE	130.189	353.15	458.00	684.00	34.60	429.0	0.3035	0.261	0.328
168	C10H10O4	DIMETHYL PHTHALATE	194.187	272.15	556.85	766.00	27.80	530.0	0.3664	0.231	0.647
169	C10H10O4	DIMETHYL TEREPHTHALATE	194.187	413.80	561.15	772.00	27.80	529.0	0.3671	0.229	0.637
170	C10H12	DICYCLOPENTADIENE	132.205	307.00	443.00	660.00	30.60	445.0	0.2971	0.248	0.285
171	C10H12	1-2-3-4-TETRAHYDRONAPHTHALENE	132.205	237.40	480.77	720.15	36.20	441.0	0.2998	0.267	0.328
172	C10H12O	ANETHOLE	148.205	294.50	508.45	723.00	29.00	482.0	0.3075	0.233	0.485
173	C10H12O4	DIALLYL MALEATE	196.203	226.15	520.00	693.00	23.30	606.0	0.3238	0.245	0.789
174	C10H14	n-BUTYLBENZENE	134.221	185.30	456.46	660.55	28.87	497.0	0.2701	0.261	0.392
175	C10H14	sec-BUTYLBENZENE	134.221	197.72	446.48	664.54	29.51	497.0	0.2701	0.265	0.276
176	C10H14	tert-BUTYLBENZENE	134.221	215.27	442.30	660.00	29.70	492.0	0.2728	0.266	0.266
177	C10H14	m-CYMENE	134.221	209.44	448.23	657.00	29.30	485.0	0.2767	0.260	0.341
178	C10H14	o-CYMENE	134.221	201.64	451.33	662.00	29.30	489.0	0.2745	0.260	0.337
179	C10H14	p-CYMENE	134.221	205.25	450.28	653.15	28.37	492.0	0.2728	0.257	0.372
180	C10H14	m-DIETHYLBENZENE	134.221	189.26	454.29	663.00	28.80	488.0	0.2750	0.255	0.350
181	C10H14	o-DIETHYLBENZENE	134.221	241.93	456.61	668.00	28.80	502.0	0.2674	0.260	0.340
182	C10H14	p-DIETHYLBENZENE	134.221	230.32	456.94	657.96	28.03	497.0	0.2701	0.255	0.404
183	C10H14	2-ETHYL-m-XYLENE	134.221	256.89	463.19	671.00	30.20	482.0	0.2785	0.261	0.407
184	C10H14	2-ETHYL-p-XYLENE	134.221	219.52	459.98	663.00	28.80	482.0	0.2785	0.252	0.411
185	C10H14	3-ETHYL-o-XYLENE	134.221	223.64	467.11	680.00	28.80	507.0	0.2647	0.258	0.362
186	C10H14	4-ETHYL-m-XYLENE	134.221	210.27	461.59	665.00	28.80	482.0	0.2785	0.251	0.414
187	C10H14	4-ETHYL-o-XYLENE	134.221	206.22	462.93	667.00	28.80	490.0	0.2739	0.254	0.411
188	C10H14	5-ETHYL-m-XYLENE	134.221	188.82	456.93	655.00	27.50	482.0	0.2785	0.243	0.417
189	C10H14	ISOBUTYLBENZENE	134.221	221.70	445.94	650.15	30.40	456.0	0.2943	0.256	0.381
190	C10H14	1-2-3-5-TETRAMETHYLBENZENE	134.221	249.46	471.15	679.00	29.70	482.0	0.2785	0.254	0.424
191	C10H14	1-2-4-5-TETRAMETHYLBENZENE	134.221	352.38	469.99	675.15	29.38	482.0	0.2785	0.252	0.435
192	C10H14O	p-tert-BUTYLPHENOL	150.221	371.56	512.88	734.00	33.40	493.0	0.3047	0.270	0.510
193	C10H14O2	p-tert-BUTYLCATECHOL	166.220	325.00	558.00	776.00	37.70	511.0	0.3253	0.299	0.740
194	C10H15N	N-N-DIETYHLANILINE	149.236	235.15	489.42	702.00	28.50	556.0	0.2684	0.272	0.426
195	C10H15N	2-6-DIETHYLANILINE	149.236	276.65	508.65	678.00	31.20	495.0	0.3015	0.274	0.954
196	C10H16	CAMPHENE	136.237	320.15	433.65	638.00	27.50	499.0	0.2730	0.259	0.296
197	C10H16	D-LIMONENE	136.237	199.00	449.65	660.00	27.50	524.0	0.2600	0.263	0.313
198	C10H16	alpha-PHELLANDRENE	136.237	---	448.15	649.00	28.20	500.0	0.2725	0.261	0.381
199	C10H16	beta-PHELLANDRENE	136.237	---	447.15	648.00	28.20	487.0	0.2797	0.255	0.374
200	C10H16	alpha-PINENE	136.237	209.15	429.29	632.00	27.60	504.0	0.2703	0.265	0.286
201	C10H16	beta-PINENE	136.237	211.61	439.19	643.00	27.60	506.0	0.2692	0.261	0.325
202	C10H16	alpha-TERPINENE	136.237	---	450.35	652.00	28.00	506.0	0.2692	0.261	0.376
203	C10H16	gamma-TERPINENE	136.237	---	456.15	661.00	28.00	505.0	0.2698	0.257	0.375
204	C10H16	TERPINOLENE	136.237	---	458.15	672.00	27.70	509.0	0.2677	0.252	0.301
205	C10H16O	CAMPHOR	152.236	453.25	480.57	709.00	29.90	460.0	0.3309	0.233	0.319
206	C10H18	cis-DECAHYDRONANPHTALENE	138.253	230.20	468.97	702.25	32.42	480.0	0.2880	0.267	0.294
207	C10H18	trans-DECAHYDRONAPHTHALENE	138.253	242.79	460.46	687.05	28.37	480.0	0.2880	0.238	0.254
208	C10H18O4	SEBACIC ACID	202.251	407.65	642.09	815.00	23.50	658.0	0.3074	0.228	1.205
209	C10H20	n-BUTYLCYCLOHEXANE	140.269	198.42	454.13	667.00	25.70	534.0	0.2627	0.247	0.274
210	C10H20	1-DECENE	140.269	206.89	443.75	617.05	21.68	585.0	0.2398	0.247	0.465
211	C10H20O	1-DECANAL	156.268	267.15	488.15	657.00	21.50	580.0	0.2694	0.228	0.642
212	C10H20O2	n-DECANOIC ACID	172.268	304.75	543.15	713.00	22.50	600.0	0.2871	0.228	0.877
213	C10H20O2	2-ETHYLHEXYL ACETATE	172.268	180.15	471.75	639.00	21.70	600.0	0.2871	0.245	0.631
214	C10H20O2	ISOPENTYL ISOVALERATE	172.268	215.00	467.15	637.00	22.00	600.0	0.2871	0.249	0.579

NO	FORMULA	NAME	MW g/mol	T_F K	T_B K	T_C K	P_C bar	V_C cm^3/mol	ρ_C g/cm^3	Z_C	ω
215	C10H22	n-DECANE	142.285	243.49	447.30	618.45	21.23	603.1	0.2359	0.249	0.484
216	C10H22	2-2-DIMETHYLOCTANE	142.285	---	430.05	602.00	21.60	574.0	0.2479	0.248	0.429
217	C10H22	2-METHYLNONANE	142.285	198.50	440.15	610.00	21.20	583.0	0.2441	0.244	0.472
218	C10H22	3-METHYLNONANE	142.285	188.35	440.95	613.00	21.60	583.0	0.2441	0.247	0.465
219	C10H22	4-METHYLNONANE	142.285	174.45	438.85	610.00	21.60	583.0	0.2441	0.248	0.465
220	C10H22	5-METHYLNONANE	142.285	185.45	438.30	610.00	21.60	583.0	0.2441	0.248	0.456
221	C10H22O	1-DECANOL	158.284	280.05	503.35	690.00	23.70	599.6	0.2640	0.248	0.613
222	C10H22O	DI-n-PENTYL ETHER	158.284	203.72	459.90	622.00	20.90	593.0	0.2669	0.240	0.601
223	C10H22O	ISODECANOL	158.284	213.15	493.00	644.00	22.80	591.0	0.2678	0.252	0.913
224	C10H22O5	TETRAETHYLENE GLYCOL DIMETHYL ETHER	222.282	243.45	548.95	705.00	19.40	674.0	0.3298	0.223	0.965
225	C10H22S	n-DECYL MERCAPTAN	174.351	247.56	512.35	696.00	21.30	624.0	0.2794	0.230	0.588
226	C10H23N	n-DECYLAMINE	157.299	288.85	493.65	663.00	21.80	629.0	0.2501	0.249	0.669
227	C11H10	1-METHYLNAPHTHALENE	142.200	242.67	517.83	772.04	36.60	523.0	0.2719	0.298	0.348
228	C11H10	2-METHYLNAPHTHALENE	142.200	307.73	514.20	761.00	32.50	507.0	0.2805	0.260	0.346
229	C11H14O2	n-BUTYL BENZOATE	178.231	251.65	523.15	724.00	25.90	555.0	0.3211	0.239	0.575
230	C11H16	n-PENTYLBENZENE	148.248	198.15	478.61	679.90	26.04	550.0	0.2695	0.253	0.439
231	C11H16O	p-tert-AMYLPHENOL	164.247	366.00	535.15	751.00	29.80	546.0	0.3008	0.261	0.569
232	C11H20O2	2-ETHYLHEXYL ACRYLATE	184.279	183.15	489.15	655.00	20.70	639.0	0.2884	0.243	0.673
233	C11H22	1-UNDECENE	154.296	223.99	465.82	638.00	20.30	642.0	0.2403	0.246	0.517
234	C11H22O	1-UNDECANAL	170.295	273.15	506.15	672.00	20.00	632.0	0.2695	0.226	0.697
235	C11H24	n-UNDECANE	156.312	247.57	469.08	638.76	19.66	657.0	0.2379	0.243	0.536
236	C11H24O	1-UNDECANOL	172.311	289.05	518.15	704.00	20.80	643.0	0.2680	0.229	0.587
237	C11H24S	UNDECYL MERCAPTAN	188.378	270.15	530.55	710.00	19.80	676.0	0.2787	0.227	0.636
238	C12H8O	DIBENZOFURAN	168.195	355.65	557.86	837.80	32.00	533.0	0.3156	0.245	0.275
239	C12H9N	DIBENZOPYRROLE	167.210	517.95	627.86	899.00	32.60	482.0	0.3469	0.210	0.494
240	C12H10	ACENAPHTHENE	154.211	366.56	550.54	803.15	31.00	553.0	0.2789	0.257	0.381
241	C12H10	BIPHENYL	154.211	342.37	528.15	789.26	38.47	501.6	0.3075	0.294	0.366
242	C12H10O	DIPHENYL ETHER	170.211	300.02	531.46	763.00	31.30	502.8	0.3385	0.248	0.472
243	C12H11N	p-AMINODIPHENYL	169.226	326.00	575.00	817.00	32.90	539.0	0.3140	0.261	0.545
244	C12H11N	DIPHENYLAMINE	169.226	326.15	575.15	817.00	31.80	539.0	0.3140	0.252	0.530
245	C12H11N3	p-AMINOAZOBENZENE	197.240	401.00	633.00	877.00	29.00	642.0	0.3072	0.255	0.635
246	C12H11N3	1-3-DIPHENYLTRIAZENE	197.240	372.00	610.00	845.00	28.26	642.0	0.3072	0.258	0.623
247	C12H12	2-6-DIMETHYLNAPHTHALENE	156.227	384.55	535.15	777.00	31.70	520.0	0.3004	0.255	0.418
248	C12H12	2-7-DIMETHYLNAPHTHALENE	156.227	370.15	536.15	778.00	31.70	520.0	0.3004	0.255	0.420
249	C12H12	1-ETHYLNAPHTHALENE	156.227	259.34	531.48	776.00	30.00	520.0	0.3004	0.242	0.363
250	C12H12N2	p-AMINODIPHENYLAMINE	184.241	341.15	627.15	867.00	31.90	596.0	0.3091	0.264	0.694
251	C12H12N2	HYDRAZOBENZENE	184.241	404.15	573.00	792.00	30.90	556.0	0.3314	0.261	0.680
252	C12H14	1-2-3-TRIMETHYLINDENE	158.243	344.65	509.00	726.00	27.70	529.0	0.2991	0.243	0.441
253	C12H14O4	DIETHYL PHTHALATE	222.241	269.15	567.15	757.00	23.30	635.0	0.3500	0.235	0.763
254	C12H16	CYCLOHEXYLBENZENE	160.259	280.14	513.27	744.00	28.80	555.1	0.2887	0.258	0.379
255	C12H18	m-DIISOPROPYLBENZENE	162.275	210.02	476.33	684.00	24.50	600.0	0.2705	0.258	0.359
256	C12H18	p-DIISOPROPYLBENZENE	162.275	256.08	483.65	689.00	24.50	598.0	0.2714	0.256	0.390
257	C12H18	n-HEXYLBENZENE	162.275	212.00	499.26	698.00	23.80	618.0	0.2626	0.253	0.478
258	C12H20O4	DIBUTYL MALEATE	228.288	188.15	553.15	716.00	19.00	719.0	0.3175	0.229	0.899
259	C12H22	BICYCLOHEXYL	166.307	276.78	512.19	727.00	25.60	598.0	0.2781	0.253	0.428
260	C12H23N	DICYCLOHEXYLAMINE	181.321	273.05	529.00	737.00	25.20	619.0	0.2929	0.255	0.513
261	C12H24	1-DODECENE	168.323	237.93	486.50	657.00	18.90	700.0	0.2405	0.242	0.564
262	C12H24O	1-DODECANAL	184.322	285.15	523.15	685.00	18.60	685.0	0.2691	0.224	0.754
263	C12H24O2	n-DODECANOIC ACID	200.321	317.15	571.85	734.00	19.40	705.0	0.2841	0.224	0.967
264	C12H26	n-DODECANE	170.338	263.57	489.47	658.20	18.24	726.8	0.2344	0.242	0.573
265	C12H26O	DI-n-HEXYL ETHER	186.338	230.15	498.85	658.00	18.16	698.0	0.2670	0.232	0.711
266	C12H26O	1-DODECANOL	186.338	296.95	535.00	721.00	19.30	696.0	0.2677	0.224	0.639
267	C12H26O3	DIETHYLENE GLYCOL DI-n-BUTYL ETHER	218.337	212.95	529.15	680.00	17.60	803.0	0.2719	0.250	0.846
268	C12H26S	n-DODECYL MERCAPTAN	202.404	265.15	547.75	724.00	18.40	729.0	0.2776	0.223	0.677
269	C12H27BO3	TRI-n-BUTYL BORATE	230.156	203.15	506.65	743.15	19.89	863.3	0.2666	0.278	0.189
270	C12H27N	DODECYLAMINE	185.353	301.47	532.35	696.00	18.80	735.0	0.2522	0.239	0.769
271	C12H27N	TRI-n-BUTYLAMINE	185.353	203.00	487.15	644.00	18.00	735.0	0.2522	0.247	0.694
272	C13H10	FLUORENE	166.222	387.94	570.44	870.00	47.00	400.0	0.4156	0.260	0.349
273	C13H10O	BENZOPHENONE	182.222	321.35	579.24	816.00	30.10	591.0	0.3083	0.262	0.545
274	C13H12	DIPHENYLMETHANE	168.238	298.39	537.42	768.00	29.20	547.0	0.3076	0.250	0.462
275	C13H20	n-HEPTYLBENZENE	176.302	225.15	519.25	714.00	21.80	648.0	0.2721	0.238	0.529
276	C13H26	1-TRIDECENE	182.349	250.08	505.93	675.00	17.70	756.0	0.2412	0.238	0.612
277	C13H26O	1-TRIDECANAL	198.349	288.15	540.15	700.00	17.40	738.0	0.2688	0.221	0.785
278	C13H26O2	n-BUTYL NONANOATE	214.348	235.15	503.00	652.00	17.40	794.0	0.2700	0.255	0.828
279	C13H26O2	METHYL DODECANOATE	214.348	278.15	540.00	712.00	17.40	758.0	0.2828	0.223	0.690
280	C13H28	n-TRIDECANE	184.365	267.76	508.62	675.80	17.23	770.0	0.2394	0.236	0.619
281	C13H28O	1-TRIDECANOL	200.365	303.75	547.15	731.00	18.10	749.0	0.2675	0.223	0.627
282	C14H8O2	ANTHRAQUINONE	208.216	559.15	653.05	900.00	31.50	544.0	0.3828	0.229	0.681
283	C14H10	ANTHRACENE	178.233	489.25	615.18	873.00	29.00	554.0	0.3217	0.221	0.489
284	C14H10	DIPHENYLACETYLENE	178.233	335.65	573.00	832.00	29.00	611.0	0.2917	0.256	0.384
285	C14H10	PHENANTHRENE	178.233	372.38	613.45	869.25	29.00	554.0	0.3217	0.222	0.495
286	C14H12	cis-STILBENE	180.249	268.15	535.00	757.00	27.40	584.0	0.3086	0.254	0.471
287	C14H12	trans-STILBENE	180.249	397.35	579.65	820.00	27.40	578.0	0.3118	0.232	0.490
288	C14H12O2	BENZYL BENZOATE	212.248	292.55	596.65	820.00	25.80	694.0	0.3058	0.263	0.623
289	C14H14	1-1-DIPHENYLETHANE	182.265	255.20	545.78	775.00	26.80	604.0	0.3018	0.251	0.457

NO	FORMULA	NAME	MW g/mol	T_F K	T_B K	T_C K	P_C bar	V_C cm^3/mol	ρ_C g/cm^3	Z_C	ω
290	C14H14	1-2-DIPHENYLETHANE	182.265	324.34	553.65	780.00	26.50	606.0	0.3008	0.248	0.489
291	C14H14O	DIBENZYL ETHER	198.265	276.75	561.45	777.00	25.60	608.0	0.3261	0.241	0.591
292	C14H16	1-n-BUTYLNAPHTHALENE	184.281	253.43	562.54	792.00	26.80	631.0	0.2920	0.257	0.495
293	C14H22	n-OCTYLBENZENE	190.329	237.15	537.55	729.00	20.20	703.0	0.2707	0.234	0.572
294	C14H22O	p-tert-OCTYLPHENOL	206.328	358.55	563.60	765.00	22.80	704.0	0.2931	0.252	0.631
295	C14H28	1-TETRADECENE	196.376	260.30	524.25	692.00	16.60	817.0	0.2404	0.236	0.648
296	C14H28O2	n-TETRADECANOIC ACID	228.375	327.55	599.35	756.00	17.00	811.0	0.2816	0.219	1.025
297	C14H30	n-TETRADECANE	198.392	279.01	526.73	692.40	16.21	842.8	0.2354	0.237	0.662
298	C14H30O	1-TETRADECANOL	214.392	310.65	560.15	741.00	17.00	802.0	0.2673	0.221	0.677
299	C14H31N	TETRADECYLAMINE	213.407	311.34	564.45	722.30	16.60	887.0	0.2406	0.245	0.860
300	C15H10N2O2	DIPHENYLMETHANE-4-4'-DIISOCYANATE	250.257	311.20	609.00	802.00	22.80	712.0	0.3515	0.243	0.950
301	C15H16O	p-CUMYLPHENOL	212.291	346.00	608.15	834.00	26.80	659.0	0.3221	0.255	0.660
302	C15H16O2	BISPHENOL A	228.291	426.15	633.65	849.00	29.30	677.0	0.3372	0.281	0.945
303	C15H24	n-NONYLBENZENE	204.356	249.00	555.20	741.00	18.95	790.0	0.2587	0.243	0.638
304	C15H24O	2-6-DI-tert-BUTYL-p-CRESOL	220.355	344.00	538.00	720.00	21.10	757.0	0.2911	0.267	0.686
305	C15H24O	NONYLPHENOL	220.355	---	581.00	757.00	20.70	757.0	0.2911	0.249	0.900
306	C15H30	1-PENTADECENE	210.403	269.42	541.61	708.00	15.70	875.0	0.2405	0.233	0.684
307	C15H30O2	PENTADECANOIC ACID	242.402	325.68	612.05	766.00	16.00	864.0	0.2806	0.217	1.040
308	C15H32	n-PENTADECANE	212.419	283.11	543.83	706.80	15.20	880.0	0.2414	0.228	0.705
309	C16H10	FLUORANTHENE	202.255	383.33	655.95	905.00	26.10	655.0	0.3088	0.227	0.588
310	C16H10	PYRENE	202.255	423.81	667.95	936.00	26.10	630.0	0.3210	0.211	0.509
311	C16H12	1-PHENYLNAPHTHALENE	204.271	318.15	607.15	849.00	26.30	656.0	0.3114	0.244	0.531
312	C16H20	1-n-HEXYLNAPHTHALENE	212.335	255.15	595.15	813.00	22.50	741.0	0.2866	0.247	0.587
313	C16H22O4	DIBUTYL PHTHALATE	278.348	238.15	613.15	781.00	17.50	846.0	0.3290	0.228	0.947
314	C16H26	n-DECYLBENZENE	218.382	258.77	571.04	753.00	17.70	881.0	0.2479	0.249	0.681
315	C16H32	n-DECYLCYCLOHEXANE	224.430	271.42	570.75	751.25	16.50	858.0	0.2616	0.227	0.663
316	C16H32	1-HEXADECENE	224.430	277.51	558.02	722.00	14.80	933.0	0.2405	0.230	0.732
317	C16H32O2	n-HEXADECANOIC ACID	256.429	335.95	624.15	776.00	15.10	917.0	0.2796	0.215	1.083
318	C16H34	n-HEXADECANE	226.446	291.34	560.01	720.60	14.19	930.0	0.2435	0.220	0.747
319	C16H34O	DI-n-OCTYL ETHER	242.445	265.55	559.65	707.00	14.40	910.0	0.2664	0.223	0.934
320	C16H34O	1-HEXADECANOL	242.445	322.35	585.15	761.00	15.10	907.0	0.2673	0.216	0.748
321	C17H28	n-UNDECYLBENZENE	232.409	268.00	586.40	764.00	16.72	910.0	0.2554	0.240	0.738
322	C17H34	1-HEPTADECENE	238.457	284.40	573.48	736.00	14.10	955.0	0.2497	0.220	0.753
323	C17H36	n-HEPTADECANE	240.473	295.13	575.30	733.37	13.17	1005.8	0.2391	0.217	0.768
324	C17H36O	1-HEPTADECANOL	256.472	327.05	597.15	770.00	14.30	960.0	0.2672	0.214	0.795
325	C18H12	CHRYSENE	228.293	531.15	714.15	979.00	23.90	690.0	0.3309	0.213	0.604
326	C18H14	m-TERPHENYL	230.309	360.00	650.00	924.85	35.06	767.7	0.3000	0.350	0.558
327	C18H14	o-TERPHENYL	230.309	329.35	609.00	890.95	39.01	752.6	0.3060	0.396	0.467
328	C18H14	p-TERPHENYL	230.309	485.00	649.15	925.95	33.24	762.6	0.3020	0.329	0.528
329	C18H15P	TRIPHENYLPHOSPHINE	262.291	354.40	650.15	1008.00	78.40	554.0	0.4734	0.518	0.452
330	C18H15O4P	TRIPHENYL PHOSPHATE	326.288	323.15	686.65	---	---	---	---	---	---
331	C18H16N2	N-N'-DIPHENYL-p-PHENYLENEDIAMINE	260.339	409.00	688.00	906.00	23.10	817.0	0.3187	0.251	0.876
332	C18H22	2-3-DIMETHYL-2-3-DIPHENYLBUTANE	238.373	392.15	589.00	805.00	19.90	781.0	0.3052	0.232	0.521
333	C18H22O2	DICUMYL PEROXIDE	270.371	311.15	669.00	884.00	21.80	873.0	0.3097	0.259	0.450
334	C18H30	n-DODECYLBENZENE	246.436	275.93	600.76	774.26	15.79	1000.0	0.2464	0.245	0.786
335	C18H32O2	LINOLEIC ACID	280.451	268.15	628.00	775.00	14.10	990.0	0.2833	0.217	1.176
336	C18H34O2	OLEIC ACID	282.467	286.53	633.00	781.00	13.90	1000.0	0.2825	0.214	1.187
337	C18H34O4	DIBUTYL SEBACATE	314.466	263.95	622.15	768.00	13.20	1050.0	0.2995	0.217	1.126
338	C18H34O4	DIHEXYL ADIPATE	314.466	259.35	621.15	767.00	13.20	1030.0	0.3053	0.213	1.094
339	C18H36	1-OCTADECENE	252.484	290.76	587.97	748.00	13.40	1050.0	0.2405	0.226	0.790
340	C18H36O2	STEARIC ACID	284.483	342.75	648.35	799.00	13.60	1020.0	0.2789	0.209	1.084
341	C18H38	n-OCTADECANE	254.500	301.33	589.86	745.26	12.14	1070.0	0.2379	0.210	0.795
342	C18H38O	DINONYL ETHER	270.499	---	591.00	736.00	13.00	1020.0	0.2652	0.217	1.002
343	C18H38O	1-OCTADECANOL	270.499	331.05	608.15	777.00	13.60	1010.0	0.2678	0.213	0.863
344	C19H26	1-n-NONYLNAPHTHALENE	254.415	284.15	639.00	849.00	16.80	1000.0	0.2544	0.238	0.617
345	C19H32	n-TRIDECYLBENZENE	260.463	283.15	614.43	783.00	15.00	1060.0	0.2457	0.244	0.844
346	C19H36O2	METHYL OLEATE	296.494	293.05	617.00	764.00	12.80	1060.0	0.2797	0.214	1.049
347	C19H38	1-NONADECENE	266.511	296.55	602.17	760.00	12.80	1100.0	0.2423	0.223	0.841
348	C19H38O2	NONADECANOIC ACID	298.510	341.23	659.15	810.00	13.00	1080.0	0.2764	0.208	1.070
349	C19H40	n-NONADECANE	268.527	305.33	603.05	755.93	11.17	1130.0	0.2376	0.201	0.820
350	C20H16	TRIPHENYLETHYLENE	256.347	342.15	669.00	908.00	21.00	860.0	0.2981	0.239	0.600
351	C20H28	1-n-DECYLNAPHTHALENE	268.442	288.15	652.00	859.00	15.80	1070.0	0.2509	0.237	0.642
352	C20H30O2	ABIETIC ACID	302.457	446.65	649.70	832.00	16.80	930.0	0.3252	0.226	1.129
353	C20H31N	DEHYDROABIETYLAMINE	285.473	317.65	660.00	863.00	17.00	1020.0	0.2799	0.242	0.742
354	C20H40	1-EICOSENE	280.538	301.76	615.54	771.00	12.20	1160.0	0.2418	0.221	0.877
355	C20H42	n-EICOSANE	282.553	309.59	616.93	767.04	10.40	1190.0	0.2374	0.194	0.876
356	C20H42O	1-EICOSANOL	298.553	338.55	629.15	792.00	12.40	1120.0	0.2666	0.211	0.937
357	C21H21O4P	TRI-o-CRESYL PHOSPHATE	368.369	240.15	---	---	---	---	---	---	---
358	C22H44O2	n-BUTYL STEARATE	340.590	299.45	623.15	764.00	11.10	1230.0	0.2769	0.215	1.035
359	C24H38O4	DIISOOCTYL PHTHALATE	390.563	---	694.00	851.00	11.80	1420.0	0.2750	0.237	1.088
360	C24H38O4	DIOCTYL PHTHALATE	390.563	223.15	657.15	806.00	11.80	1270.0	0.3075	0.224	1.142
361	C24H42O	DINONYLPHENOL	346.597	---	722.00	886.00	12.40	1220.0	0.2841	0.205	1.136
362	C26H20	TETRAPHENYLETHYLENE	332.445	496.15	760.00	996.00	17.10	1020.0	0.3259	0.211	0.729
363	C28H46O4	DIISODECYL PHTHALATE	446.671	227.59	723.00	887.00	10.00	1460.0	0.3059	0.198	1.076

Appendix E

GAS HEAT CAPACITY FOR C_8 TO C_{28} COMPOUNDS

Carl L. Yaws
Lamar University, Beaumont, Texas

$C_p = A + B\,T + C\,T^2 + D\,T^3 + E\,T^4$ (C_p - joule/g-mol K, T - K)

NO	FORMULA	NAME	A	B	C	D	E	TMIN	TMAX
1	C8H4Cl2O2	ISOPHTHALOYL CHLORIDE	32.762	5.2222E-01	-3.3597E-04	9.0843E-08	-9.2349E-12	298	1200
2	C8H4O3	PHTHALIC ANHYDRIDE	40.083	3.6084E-02	9.5956E-04	-1.2341E-06	4.6597E-10	298	1000
3	C8H6O4	ISOPHTHALIC ACID	-48.374	6.9316E-01	-4.1468E-04	7.2676E-08	8.1593E-12	298	1500
4	C8H6O4	PHTHALIC ACID	-48.374	6.9316E-01	-4.1468E-04	7.2676E-08	8.1593E-12	298	1500
5	C8H6O4	TEREPHTHALIC ACID	-48.374	6.9316E-01	-4.1468E-04	7.2676E-08	8.1593E-12	298	1500
6	C8H6S	BENZOTHIOPHENE	-47.900	8.1457E-01	-8.0881E-04	4.1421E-07	-8.5298E-11	298	1500
7	C8H7N	INDOLE	-46.384	7.0422E-01	-5.3462E-04	1.9548E-07	-2.7036E-11	200	1500
8	C8H8	STYRENE	71.201	5.4767E-02	6.4793E-04	-6.9875E-07	2.1232E-10	100	1500
9	C8H8O	ACETOPHENONE	-44.384	6.3161E-01	-3.8644E-04	9.1755E-08	-2.9424E-12	298	1500
10	C8H8O	p-TOLUALDEHYDE	-34.314	6.9270E-01	-5.3448E-04	1.9482E-07	-1.6767E-11	298	1200
11	C8H8O2	METHYL BENZOATE	-44.363	6.6062E-01	-3.0730E-04	-7.6698E-08	7.8555E-11	298	1200
12	C8H8O2	o-TOLUIC ACID	5.831	3.2470E-01	4.8726E-04	-8.7808E-07	3.7290E-10	298	1000
13	C8H8O2	p-TOLUIC ACID	5.831	3.2470E-01	4.8726E-04	-8.7808E-07	3.7290E-10	298	1000
14	C8H8O3	METHYL SALICYLATE	-64.438	9.2054E-01	-8.6046E-04	4.1813E-07	-8.1500E-11	298	1500
15	C8H8O3	VANILLIN	-24.141	7.6542E-01	-4.9618E-04	1.3823E-07	-1.9509E-11	298	1200
16	C8H9NO	ACETANILIDE	-52.405	7.8304E-01	-5.9239E-04	2.3324E-07	-4.1725E-11	298	1500
17	C8H10	ETHYLBENZENE	-20.527	5.9578E-01	-3.0849E-04	3.5621E-08	1.2409E-11	200	1500
18	C8H10	m-XYLENE	-16.725	5.6424E-01	-2.6465E-04	1.3381E-08	1.5869E-11	200	1500
19	C8H10	o-XYLENE	0.182	5.1344E-01	-2.0212E-04	-2.1615E-08	2.3212E-11	200	1500
20	C8H10	p-XYLENE	-17.360	5.6470E-01	-2.6293E-04	1.1217E-08	1.6544E-11	200	1500
21	C8H10O	m-ETHYLPHENOL	17.179	5.1321E-01	-1.5178E-04	-9.7687E-08	5.1382E-11	200	1500
22	C8H10O	p-ETHYLPHENOL	17.179	5.1321E-01	-1.5178E-04	-9.7687E-08	5.1382E-11	200	1500
23	C8H10O	PHENETOLE	-70.622	8.7227E-01	-7.3933E-04	3.3808E-07	-6.7682E-11	298	1500
24	C8H10O	2-PHENYLETHANOL	-41.581	7.7144E-01	-6.0352E-04	2.4945E-07	-4.5938E-11	298	1500
25	C8H10O	2,3-XYLENOL	5.637	6.6110E-01	-4.6084E-04	1.6135E-07	-2.2812E-11	200	1500
26	C8H10O	2,4-XYLENOL	-6.981	6.8005E-01	-4.6398E-04	1.5240E-07	-1.8683E-11	200	1500
27	C8H10O	2,5-XYLENOL	-0.097	6.4699E-01	-4.0504E-04	1.0860E-07	-7.1789E-12	200	1500
28	C8H10O	2,6-XYLENOL	-3.351	6.5837E-01	-4.2958E-04	1.3046E-07	-1.3721E-11	200	1500
29	C8H10O	3,4-XYLENOL	-5.010	7.1824E-01	-5.6191E-04	2.3462E-07	-4.1599E-11	200	1500
30	C8H10O	3,5-XYLENOL	-14.573	6.9845E-01	-4.8247E-04	1.6146E-07	-2.0501E-11	200	1500
31	C8H11N	N,N-DIMETHYLANILINE	-80.587	9.3415E-01	-7.6870E-04	3.2262E-07	-5.7595E-11	298	1500
32	C8H11N	o-ETHYLANILINE	-44.119	8.6260E-01	-7.5428E-04	3.5713E-07	-7.2513E-11	298	1500
33	C8H11N	2,4,6-TRIMETHYLPYRIDINE	-44.959	7.5625E-01	-4.7616E-04	1.2070E-07	-5.5157E-12	298	1500
34	C8H11NO	p-PHENETIDINE	-61.255	9.5389E-01	-8.2789E-04	3.7816E-07	-7.4127E-11	298	1500
35	C8H12	1,5-CYCLOOCTADIENE	4.987	4.2829E-01	1.9618E-04	-4.0302E-07	1.3486E-10	100	1500
36	C8H12	VINYLCYCLOHEXENE	-85.630	9.7156E-01	-8.6793E-04	4.1915E-07	-8.4485E-11	298	1500
37	C8H12O4	1,4-CYCLOHEXANEDICARBOXYLIC ACID	-95.482	1.1417E+00	-9.0210E-04	3.5790E-07	-6.0891E-11	298	1200
38	C8H12O4	DIETHYL MALEATE	-89.669	1.5506E+00	-2.0466E-03	1.3800E-06	-3.5435E-10	298	1200
39	C8H14O2	n-BUTYL METHACRYLATE	-51.893	1.0235E+00	-9.3080E-04	4.7360E-07	-1.0396E-10	298	1200
40	C8H14O3	BUTYRIC ANHYDRIDE	29.745	7.9376E-01	-4.1894E-04	8.7715E-08	-5.9476E-12	298	1200
41	C8H14O4	DIETHYL SUCCINATE	-50.188	1.2234E+00	-1.2888E-03	7.3303E-07	-1.6796E-10	298	1500
42	C8H16	1,1-DIMETHYLCYCLOHEXANE	12.609	4.3616E-01	3.5994E-04	-5.5592E-07	1.7723E-10	200	1500
43	C8H16	cis-1,2-DIMETHYLCYCLOHEXANE	12.356	4.6185E-01	2.8460E-04	-4.9224E-07	1.6009E-10	200	1500
44	C8H16	trans-1,2-DIMETHYLCYCLOHEXANE	5.195	5.1990E-01	1.7366E-04	-4.0995E-07	1.3877E-10	200	1500
45	C8H16	cis-1,3-DIMETHYLCYCLOHEXANE	16.162	4.4120E-01	3.2552E-04	-5.2079E-07	1.6680E-10	200	1500
46	C8H16	trans-1,3-DIMETHYLCYCLOHEXANE	17.334	4.4313E-01	3.0406E-04	-5.0089E-07	1.6161E-10	200	1500
47	C8H16	cis-1,4-DIMETHYLCYCLOHEXANE	17.334	4.4313E-01	3.0406E-04	-5.0089E-07	1.6161E-10	200	1500
48	C8H16	trans-1,4-DIMETHYLCYCLOHEXANE	7.358	4.9586E-01	2.2944E-04	-4.5522E-07	1.5104E-10	200	1500
49	C8H16	ETHYLCYCLOHEXANE	9.711	4.9505E-01	2.0606E-04	-4.2645E-07	1.4166E-10	200	1500
50	C8H16	2-ETHYL-1-HEXENE	-24.228	8.3947E-01	-6.1664E-04	2.4854E-07	-4.3134E-11	298	1500
51	C8H16	1-METHYL-1-ETHYLCYCLOPENTANE	-69.713	9.2602E-01	-6.2526E-04	2.0490E-07	-2.4889E-11	298	1500
52	C8H16	1-OCTENE	56.266	4.0665E-01	1.5805E-04	-3.2277E-07	1.0600E-10	200	1500
53	C8H16	trans-2-OCTENE	6.815	6.4056E-01	-2.3322E-04	-4.6067E-08	3.3079E-11	200	1500
54	C8H16	trans-3-OCTENE	-5.979	6.9800E-01	-3.1979E-04	9.4308E-09	1.9956E-11	200	1500
55	C8H16	trans-4-OCTENE	-5.979	6.9800E-01	-3.1979E-04	9.4308E-09	1.9956E-11	200	1500
56	C8H16	n-PROPYLCYCLOPENTANE	-51.866	7.8827E-01	-3.5255E-04	-6.8545E-09	3.1314E-11	100	1500
57	C8H16	2,4,4-TRIMETHYL-1-PENTENE	-28.020	8.6749E-01	-6.3580E-04	2.4452E-07	-3.9076E-11	298	1500
58	C8H16	2,4,4-TRIMETHYL-2-PENTENE	-23.378	8.4303E-01	-6.1037E-04	2.3775E-07	-3.9769E-11	298	1500
59	C8H16O	2-ETHYLHEXANAL	-30.667	8.9033E-01	-6.5620E-04	2.6358E-07	-4.4888E-11	298	1500
60	C8H16O	1-OCTANAL	85.407	3.0880E-01	4.0878E-04	-5.4231E-07	1.6932E-10	200	1500
61	C8H16O	2-OCTANONE	81.259	3.2148E-01	3.8818E-04	-5.4646E-07	1.7288E-10	150	1500
62	C8H16O2	n-BUTYL n-BUTYRATE	14.674	7.8762E-01	-3.9225E-04	4.2787E-08	1.5217E-11	298	1200

NO	FORMULA	NAME	$C_p = A + B T + C T^2 + D T^3 + E T^4$ (A	B	C	D	E)	TMIN	TMAX
63	C8H16O2	n-HEXYL ACETATE	-46.949	1.0667E+00	-9.5577E-04	4.7655E-07	-9.8701E-11	298	1500
64	C8H16O2	ISOBUTYL ISOBUTYRATE	-78.711	1.1911E+00	-1.1320E-03	5.8376E-07	-1.2228E-10	298	1500
65	C8H16O2	n-OCTANOIC ACID	-20.242	9.9093E-01	-9.2370E-04	5.5027E-07	-1.5434E-10	298	1000
66	C8H16O4	DIETHYLENE GLYCOL ETHYL ETHER ACETATE	-51.637	1.1924E+00	-1.0849E-03	5.3285E-07	-1.0908E-10	298	1500
67	C8H18	2,2-DIMETHYLHEXANE	-9.102	7.9198E-01	-4.3438E-04	1.1094E-07	-9.1975E-12	200	1500
68	C8H18	2,3-DIMETHYLHEXANE	-45.246	9.7125E-01	-7.6224E-04	3.4891E-07	-7.0688E-11	200	1500
69	C8H18	2,4-DIMETHYLHEXANE	-35.844	9.7252E-01	-7.9337E-04	3.8126E-07	-8.0700E-11	200	1500
70	C8H18	2,5-DIMETHYLHEXANE	-32.363	9.0722E-01	-6.5105E-04	2.6842E-07	-4.9960E-11	200	1500
71	C8H18	3,3-DIMETHYLHEXANE	-37.306	9.6180E-01	-7.3386E-04	3.2761E-07	-6.5298E-11	200	1500
72	C8H18	3,4-DIMETHYLHEXANE	-59.720	1.0415E+00	-8.8492E-04	4.3894E-07	-9.4154E-11	200	1500
73	C8H18	3-ETHYLHEXANE	16.214	6.6412E-01	-2.2656E-04	-5.1790E-08	3.5344E-11	200	1500
74	C8H18	3-ETHYL-2-METHYLPENTANE	-7.477	7.7747E-01	-4.2844E-04	9.1763E-08	0.0000E+00	298	1000
75	C8H18	2-METHYLHEPTANE	-3.367	7.5824E-01	-3.8216E-04	5.7358E-08	8.0178E-12	200	1500
76	C8H18	3-METHYLHEPTANE	-10.106	7.8711E-01	-4.3415E-04	9.7487E-08	-2.9023E-12	200	1500
77	C8H18	4-METHYLHEPTANE	-17.581	8.3526E-01	-5.1418E-04	1.5104E-07	-1.5855E-11	200	1500
78	C8H18	n-OCTANE	29.053	5.8016E-01	-5.7103E-05	-1.9548E-07	7.6614E-11	200	1500
79	C8H18	2,2,3-TRIMETHYLPENTANE	-48.847	9.9777E-01	-8.0693E-04	3.9894E-07	-8.7211E-11	200	1500
80	C8H18	2,2,4-TRIMETHYLPENTANE	-21.703	8.5849E-01	-5.5323E-04	2.0892E-07	-3.7285E-11	200	1500
81	C8H18	2,3,3-TRIMETHYLPENTANE	-51.678	1.0143E+00	-8.2601E-04	4.0855E-07	-8.9531E-11	200	1500
82	C8H18	2,3,4-TRIMETHYLPENTANE	-53.615	1.0646E+00	-9.6734E-04	5.2516E-07	-1.2149E-10	200	1500
83	C8H18O	DI-n-BUTYL ETHER	86.995	3.4274E-01	3.7493E-04	-5.7832E-07	1.8911E-10	200	1500
84	C8H18O	DI-sec-BUTYL ETHER	-50.577	1.1014E+00	-9.9402E-04	5.1326E-07	-1.1304E-10	298	1200
85	C8H18O	DI-tert-BUTYL ETHER	122.563	1.7324E-01	6.4796E-04	-6.9227E-07	2.0237E-10	200	1500
86	C8H18O	2-ETHYL-1-HEXANOL	-8.577	8.3851E-01	-5.0979E-04	1.4511E-07	-1.4766E-11	298	1500
87	C8H18O	1-OCTANOL	13.196	7.2493E-01	-2.7623E-04	-5.8380E-08	4.5179E-11	200	1500
88	C8H18O	2-OCTANOL	-23.930	9.4474E-01	-7.0058E-04	2.8277E-07	-4.9163E-11	298	1500
89	C8H18O2	DI-t-BUTYL PEROXIDE	-5.907	9.4614E-01	-6.7505E-04	2.4895E-07	-3.9188E-11	298	1500
90	C8H18O2S	DI-n-BUTYL SULFONE	6.590	9.1442E-01	-5.5866E-04	1.7288E-07	-1.9647E-11	298	1500
91	C8H18O3	DIETHYLENE GLYCOL DIETHYL ETHER	-31.678	1.0594E+00	-8.1318E-04	3.3723E-07	-6.1289E-11	298	1500
92	C8H18O3	DIETHYLENE GLYCOL MONOBUTYL EHTER	-15.996	9.8794E-01	-6.9921E-04	2.5671E-07	-4.0681E-11	298	1500
93	C8H18O4	TRIETHYLENE GLYCOL DIMETHYL ETHER	-15.847	1.0394E+00	-7.4905E-04	2.8115E-07	-4.5915E-11	298	1500
94	C8H18O5	TETRAETHYLENE GLYCOL	7.854	1.0016E+00	-7.0468E-04	2.6794E-07	-4.8409E-11	298	1200
95	C8H18S	n-OCTYL MERCAPTAN	63.070	4.9322E-01	1.4077E-04	-3.4436E-07	1.1448E-10	200	1500
96	C8H18S	tert-OCTYL MERCAPTAN	-27.449	1.0002E+00	-7.2696E-04	2.4916E-07	-3.1819E-11	298	1500
97	C8H19N	DI-n-BUTYLAMINE	-36.248	1.0025E+00	-7.6232E-04	3.2620E-07	-6.0071E-11	298	1500
98	C8H19N	DIISOBUTYLAMINE	-37.761	9.8864E-01	-6.9887E-04	2.6003E-07	-4.1045E-11	298	1500
99	C8H19N	n-OCTYLAMINE	-11.736	9.0057E-01	-6.1188E-04	2.2599E-07	-3.5786E-11	298	1500
100	C8H23N5	TETRAETHYLENEPENTAMINE	-49.208	1.3828E+00	-1.1462E-03	5.2201E-07	-1.0064E-10	298	1500
101	C8H24O4Si4	OCTAMETHYLCYCLOTETRASILOXANE	-10.762	1.3722E+00	-8.6662E-04	2.2799E-07	-1.4708E-11	298	1500
102	C9H4O5	TRIMELLITIC ANHYDRIDE	-13.209	5.6342E-01	1.4947E-05	-4.4215E-07	2.1578E-10	298	1000
103	C9H6N2O2	TOLUENE DIISOCYANATE	-5.078	5.7582E-01	2.9402E-04	-9.0683E-07	4.3055E-10	298	1000
104	C9H7N	ISOQUINOLINE	-18.255	5.8698E-01	-2.5163E-04	-4.1653E-08	3.9647E-11	200	1500
105	C9H7N	QUINOLINE	-21.558	6.0838E-01	-2.9061E-04	-1.2260E-08	3.1722E-11	200	1500
106	C9H7NO	8-HYDROXYQUINOLINE	-62.510	9.7219E-01	-9.3439E-04	4.4959E-07	-8.6601E-11	298	1500
107	C9H8	INDENE	-31.858	6.2986E-01	-3.6332E-04	6.8279E-08	4.9422E-12	200	1500
108	C9H8O	2-METHYLBENZOFURAN	-59.800	8.8351E-01	-8.0230E-04	3.7939E-07	-7.2950E-11	298	1500
109	C9H10	INDANE	-132.570	1.1568E+00	-1.2134E-03	6.6759E-07	-1.4627E-10	298	1500
110	C9H10	alpha-METHYLSTYRENE	24.923	4.3818E-01	-1.3764E-05	-1.8472E-07	7.0450E-11	200	1500
111	C9H10	m-METHYLSTYRENE	25.882	4.3319E-01	-5.1049E-06	-1.9087E-07	7.1985E-11	200	1500
112	C9H10	o-METHYLSTYRENE	25.882	4.3319E-01	-5.1049E-06	-1.9087E-07	7.1985E-11	200	1500
113	C9H10	p-METHYLSTYRENE	25.882	4.3319E-01	-5.1049E-06	-1.9087E-07	7.1985E-11	200	1500
114	C9H10O2	BENZYL ACETATE	-64.296	9.7745E-01	-8.0623E-04	2.7233E-07	-1.0633E-12	298	1200
115	C9H10O2	ETHYL BENZOATE	-91.208	1.0326E+00	-9.5250E-04	4.6492E-07	-9.0498E-11	298	1500
116	C9H10O3	ETHYL VANILLIN	-34.060	9.0152E-01	-6.1072E-04	1.8656E-07	-2.7428E-11	298	1200
117	C9H11NO	p-DIMETHYLAMINOBENZALDEHYDE	-65.931	9.6897E-01	-6.6584E-04	1.8803E-07	-1.2951E-11	298	1500
118	C9H12	CUMENE	10.149	5.1138E-01	-1.7703E-05	-2.2612E-07	8.8002E-11	200	1500
119	C9H12	m-ETHYLTOLUENE	-7.269	5.9696E-01	-2.0235E-04	-6.2005E-08	3.8692E-11	200	1500
120	C9H12	o-ETHYLTOLUENE	8.688	5.5216E-01	-1.5746E-04	-7.9142E-08	4.0458E-11	200	1500
121	C9H12	p-ETHYLTOLUENE	-13.082	6.3055E-01	-2.5570E-04	-2.7145E-08	3.0472E-11	200	1500
122	C9H12	MESITYLENE	-8.737	6.0394E-01	-2.3025E-04	-3.1411E-08	2.8748E-11	200	1500
123	C9H12	n-PROPYLBENZENE	-10.933	6.4349E-01	-2.7829E-04	-1.4431E-08	2.8143E-11	200	1500
124	C9H12	1,2,3-TRIMETHYLBENZENE	12.802	5.5862E-01	-1.9088E-04	-4.5260E-08	2.9986E-11	200	1500
125	C9H12	1,2,4-TRIMETHYLBENZENE	7.238	5.5929E-01	-1.7851E-04	-5.9043E-08	3.4337E-11	200	1500
126	C9H12O	BENZYL ETHYL ETHER	-77.310	9.9168E-01	-8.2953E-04	3.7784E-07	-7.6033E-11	298	1500
127	C9H12O	2-PHENYL-2-PROPANOL	-42.729	8.6797E-01	-6.3040E-04	2.1037E-07	-2.1293E-11	298	1200
128	C9H12O2	CUMENE HYDROPEROXIDE	-42.988	9.9727E-01	-9.1932E-04	4.9051E-07	-1.1852E-10	298	1200
129	C9H14O	ISOPHORONE	-74.479	1.1286E+00	-1.0642E-03	5.8129E-07	-1.4417E-10	298	1200
130	C9H14O6	GLYCERYL TRIACETATE	-94.112	1.5807E+00	-1.7308E-03	9.5867E-07	-2.0165E-10	298	1200
131	C9H16O4	AZELAIC ACID	-10.832	1.1553E+00	-1.1558E-03	7.2207E-07	-2.0666E-10	298	1200
132	C9H18	ISOPROPYLCYCLOHEXANE	-72.808	1.0165E+00	-6.2550E-04	1.7248E-07	-1.4751E-11	298	1500
133	C9H18	1-NONENE	55.655	4.9879E-01	1.0927E-04	-3.1474E-07	1.0691E-10	200	1500
134	C9H18	n-PROPYLCYCLOHEXANE	25.567	5.2828E-01	2.3719E-04	-4.6758E-07	1.5413E-10	200	1500

$C_P = A + B\,T + C\,T^2 + D\,T^3 + E\,T^4$ (C_P - joule/g-mol K, T - K)

NO	FORMULA	NAME	A	B	C	D	E	TMIN	TMAX
135	C9H18O	DIISOBUTYL KETONE	-1.433	8.8406E-01	-5.7459E-04	1.9432E-07	-2.8451E-11	298	1500
136	C9H18O	1-NONANAL	84.758	3.9995E-01	3.6567E-04	-5.3736E-07	1.6751E-10	200	1500
137	C9H18O2	n-BUTYL VALERATE	-43.663	1.1626E+00	-1.0255E-03	5.0332E-07	-1.0407E-10	298	1500
138	C9H18O2	n-NONANOIC ACID	16.182	8.4306E-01	-4.3510E-04	6.1835E-08	7.4964E-12	298	1200
139	C9H18O2	n-OCTYL FORMATE	-38.335	1.1242E+00	-9.4618E-04	4.4200E-07	-8.6768E-11	298	1500
140	C9H20	3,3-DIETHYLPENTANE	37.793	6.5813E-01	-9.9686E-05	-1.5751E-07	6.2352E-11	150	1500
141	C9H20	2,2-DIMETHYL-3-ETHYLPENTANE	24.550	6.2909E-01	3.7947E-05	-2.9127E-07	1.0305E-10	150	1500
142	C9H20	2,4-DIMETHYL-3-ETHYLPENTANE	6.652	7.6279E-01	-2.3975E-04	-7.9564E-08	4.7011E-11	150	1500
143	C9H20	2,2-DIMETHYLHEPTANE	43.712	5.7185E-01	1.2970E-04	-3.6900E-07	1.2607E-10	150	1500
144	C9H20	2,6-DIMETHYLHEPTANE	15.557	7.2025E-01	-1.4814E-04	-1.6638E-07	7.3518E-11	150	1500
145	C9H20	3-ETHYLHEPTANE	68.581	4.4754E-01	3.1908E-04	-5.1182E-07	1.6482E-10	150	1500
146	C9H20	2-METHYLOCTANE	51.299	5.3562E-01	1.6961E-04	-4.0233E-07	1.3567E-10	150	1500
147	C9H20	3-METHYLOCTANE	43.182	5.7408E-01	1.0042E-04	-3.4988E-07	1.2161E-10	150	1500
148	C9H20	4-METHYLOCTANE	37.821	6.1030E-01	3.4470E-05	-3.0208E-07	1.0936E-10	150	1500
149	C9H20	n-NONANE	29.687	6.6821E-01	-9.6492E-05	-2.0014E-07	8.2200E-11	200	1500
150	C9H20	2,2,3,3-TETRAMETHYLPENTANE	-56.144	1.1449E+00	-9.5333E-04	4.9493E-07	-1.1283E-10	200	1500
151	C9H20	2,2,3,4-TETRAMETHYLPENTANE	-6.361	8.2329E-01	-3.2768E-04	-3.3527E-09	2.4144E-11	150	1500
152	C9H20	2,2,4,4-TETRAMETHYLPENTANE	45.985	5.7438E-01	1.1062E-04	-3.1707E-07	1.0496E-10	150	1500
153	C9H20	2,2,5-TRIMETHYLHEXANE	18.986	6.8130E-01	-5.8717E-05	-2.2116E-07	8.5439E-11	150	1500
154	C9H20O	2,6-DIMETHYL-4-HEPTANOL	-26.633	1.0358E+00	-7.3051E-04	2.6868E-07	-4.1207E-11	298	1500
155	C9H20O	1-NONANOL	13.919	8.1238E-01	-3.1365E-04	-6.4537E-08	5.1036E-11	200	1500
156	C9H20O	2-NONANOL	-15.877	9.8909E-01	-6.6014E-04	2.1150E-07	-1.9683E-11	298	1200
157	C9H20S	n-NONYL MERCAPTAN	66.762	5.6153E-01	1.4375E-04	-3.8391E-07	1.2953E-10	200	1500
158	C9H21N	n-NONYLAMINE	-12.915	9.9952E-01	-6.8214E-04	2.5663E-07	-4.1988E-11	298	1500
159	C9H21N	TRIPROPYLAMINE	-46.899	1.1357E+00	-8.4797E-04	3.3979E-07	-5.7551E-11	298	1500
160	C10H6O8	PYROMELLITIC ACID	-67.161	9.7245E-01	-6.8626E-04	1.9256E-07	-6.0900E-13	298	1500
161	C10H7Br	1-BROMONAPHTHALENE	-46.005	8.5830E-01	-7.4681E-04	3.2926E-07	-5.8743E-11	298	1500
162	C10H7Cl	1-CHLORONAPHTHALENE	-57.895	9.1225E-01	-8.3435E-04	3.8928E-07	-7.3276E-11	298	1500
163	C10H8	NAPHTHALENE	67.099	4.3239E-02	9.1740E-04	-1.0019E-06	3.0896E-10	50	1500
164	C10H9N	QUINALDINE	-65.789	9.5661E-01	-8.0989E-04	3.4702E-07	-6.0324E-11	298	1500
165	C10H10	m-DIVINYLBENZENE	-35.543	8.5580E-01	-7.3218E-04	3.3133E-07	-6.2061E-11	298	1500
166	C10H10	1-METHYLINDENE	-48.066	9.3476E-01	-8.3220E-04	3.8682E-07	-7.4167E-11	298	1500
167	C10H10	2-METHYLINDENE	-49.008	9.3164E-01	-8.2626E-04	3.8402E-07	-7.3411E-11	298	1500
168	C10H10O4	DIMETHYL PHTHALATE	-60.400	9.3881E-01	-5.4837E-04	6.5470E-09	7.7122E-11	298	1200
169	C10H10O4	DIMETHYL TEREPHTHALATE	-132.654	1.3389E+00	-1.2518E-03	4.2932E-07	2.8171E-11	298	1000
170	C10H12	DICYCLOPENTADIENE	-147.089	1.3677E+00	-1.3862E-03	7.1581E-07	-1.4513E-10	298	1500
171	C10H12	1,2,3,4-TETRAHYDRONAPHTHALENE	-51.694	8.3545E-01	-5.0119E-04	1.1368E-07	-6.7703E-13	200	1500
172	C10H12O	ANETHOLE	-45.965	9.3023E-01	-7.2535E-04	2.9642E-07	-5.0285E-11	298	1500
173	C10H12O4	DIALLYL MALEATE	-47.979	1.3810E+00	-1.5324E-03	8.8301E-07	-1.9930E-10	298	1500
174	C10H14	n-BUTYLBENZENE	26.627	5.3108E-01	3.7958E-05	-2.7954E-07	1.0200E-10	200	1500
175	C10H14	sec-BUTYLBENZENE	104.794	1.1063E-01	8.1144E-04	-8.6635E-07	2.5831E-10	200	1500
176	C10H14	tert-BUTYLBENZENE	-53.936	9.6706E-01	-7.1192E-04	2.5338E-07	-3.4001E-11	275	1500
177	C10H14	m-CYMENE	31.855	4.9392E-01	1.1261E-04	-3.3794E-07	1.1778E-10	200	1500
178	C10H14	o-CYMENE	-38.033	8.6610E-01	-5.5561E-04	1.6108E-07	-1.4651E-11	298	1500
179	C10H14	p-CYMENE	36.759	4.6194E-01	1.6776E-04	-3.7638E-07	1.2734E-10	200	1500
180	C10H14	m-DIETHYLBENZENE	24.047	5.5431E-01	-1.1581E-05	-2.4047E-07	9.0827E-11	200	1500
181	C10H14	o-DIETHYLBENZENE	34.267	5.3592E-01	-5.9210E-06	-2.3425E-07	8.7499E-11	200	1500
182	C10H14	p-DIETHYLBENZENE	28.958	5.2201E-01	4.4335E-05	-2.7933E-07	1.0033E-10	200	1500
183	C10H14	2-ETHYL-m-XYLENE	-32.782	9.0529E-01	-6.7917E-04	2.6936E-07	-4.5691E-11	298	1500
184	C10H14	2-ETHYL-p-XYLENE	-32.097	8.7204E-01	-6.1913E-04	2.2900E-07	-3.5721E-11	298	1500
185	C10H14	3-ETHYL-o-XYLENE	-37.474	9.3807E-01	-7.5782E-04	3.4813E-07	-7.3906E-11	298	1200
186	C10H14	4-ETHYL-m-XYLENE	-32.097	8.7204E-01	-6.1913E-04	2.2900E-07	-3.5721E-11	298	1500
187	C10H14	4-ETHYL-o-XYLENE	-32.097	8.7204E-01	-6.1913E-04	2.2900E-07	-3.5721E-11	298	1500
188	C10H14	5-ETHYL-m-XYLENE	-24.187	7.9716E-01	-4.8265E-04	1.3407E-07	-1.2432E-11	298	1500
189	C10H14	ISOBUTYLBENZENE	-70.878	1.0445E+00	-8.7778E-04	3.9154E-07	-7.1408E-11	298	1600
190	C10H14	1,2,3,5-TETRAMETHYLBENZENE	55.191	3.9958E-01	2.2251E-04	-3.8570E-07	1.2358E-10	150	1500
191	C10H14	1,2,4,5-TETRAMETHYLBENZENE	29.751	5.6692E-01	-1.1573E-04	-1.1468E-07	4.8575E-11	200	1500
192	C10H14O	p-tert-BUTYLPHENOL	-70.607	1.1546E+00	-1.0219E-03	4.6879E-07	-8.7947E-11	298	1500
193	C10H14O2	p-tert-BUTYLCATECHOL	-66.567	1.2468E+00	-1.1749E-03	5.7126E-07	-1.1278E-10	298	1500
194	C10H15N	N,N-DIETYHLANILINE	-103.246	1.2315E+00	-1.0695E-03	4.8560E-07	-9.0354E-11	298	1500
195	C10H15N	2,6-DIETHYLANILINE	-45.098	1.0631E+00	-8.9633E-04	4.0581E-07	-7.6550E-11	298	1500
196	C10H16	CAMPHENE	-154.624	1.3370E+00	-1.0808E-03	4.5075E-07	-7.7569E-11	298	1500
197	C10H16	D-LIMONENE	-75.119	1.1283E+00	-9.4007E-04	4.2286E-07	-7.9691E-11	298	1500
198	C10H16	alpha-PHELLANDRENE	-99.641	1.2604E+00	-1.1540E-03	5.6750E-07	-1.1500E-10	298	1500
199	C10H16	beta-PHELLANDRENE	-102.519	1.2851E+00	-1.1913E-03	5.8754E-07	-1.1834E-10	298	1500
200	C10H16	alpha-PINENE	-200.422	1.4834E+00	-1.2692E-03	5.4464E-07	-9.4071E-11	298	1500
201	C10H16	beta-PINENE	-140.815	1.3045E+00	-1.0299E-03	4.0838E-07	-6.5221E-11	298	1500
202	C10H16	alpha-TERPINENE	-49.869	1.1280E+00	-1.0188E-03	5.0169E-07	-1.0246E-10	298	1500
203	C10H16	gamma-TERPINENE	-71.384	1.2266E+00	-1.1733E-03	6.0467E-07	-1.2738E-10	298	1500
204	C10H16	TERPINOLENE	-59.866	1.0552E+00	-8.3267E-04	3.5840E-07	-6.6028E-11	298	1500
205	C10H16O	CAMPHOR	-145.746	1.3060E+00	-9.5043E-04	3.2082E-07	-3.9497E-11	298	1500
206	C10H18	cis-DECAHYDRONANPHTALENE	-22.786	6.4589E-01	1.8319E-04	-4.7868E-07	1.6380E-10	200	1500

$C_p = A + B\,T + C\,T^2 + D\,T^3 + E\,T^4$ (C_p - joule/g-mol K, T - K)

NO	FORMULA	NAME	A	B	C	D	E	TMIN	TMAX
207	C10H18	trans-DECAHYDRONAPHTHALENE	1.778	4.8130E-01	5.2802E-04	-7.6032E-07	2.4097E-10	150	1500
208	C10H18O4	SEBACIC ACID	12.334	1.0779E+00	-7.8296E-04	2.9696E-07	-4.8452E-11	298	1500
209	C10H20	n-BUTYLCYCLOHEXANE	90.421	2.3264E-01	9.4595E-04	-1.0571E-06	3.1928E-10	150	1500
210	C10H20	1-DECENE	121.553	2.0974E-01	7.8760E-04	-8.6982E-07	2.6033E-10	150	1500
211	C10H20O	1-DECANAL	210.932	-1.8370E-01	1.5621E-03	-1.4857E-06	4.2973E-10	150	1500
212	C10H20O2	n-DECANOIC ACID	16.364	9.3012E-01	-4.7163E-04	5.8799E-08	1.1477E-11	298	1200
213	C10H20O2	2-ETHYLHEXYL ACETATE	-18.921	1.1337E+00	-8.6008E-04	3.5303E-07	-6.1420E-11	298	1500
214	C10H20O2	ISOPENTYL ISOVALERATE	-49.541	1.2738E+00	-1.0883E-03	5.0965E-07	-9.9751E-11	298	1500
215	C10H22	n-DECANE	31.780	7.4489E-01	-1.0945E-04	-2.2668E-07	9.3458E-11	200	1500
216	C10H22	2,2-DIMETHYLOCTANE	50.808	6.2243E-01	1.6032E-04	-4.2638E-07	1.4566E-10	150	1500
217	C10H22	2-METHYLNONANE	57.338	5.8226E-01	2.2492E-04	-4.8905E-07	1.6519E-10	150	1500
218	C10H22	3-METHYLNONANE	49.113	6.2101E-01	1.5367E-04	-4.3414E-07	1.5034E-10	150	1500
219	C10H22	4-METHYLNONANE	43.716	6.5491E-01	9.6751E-05	-3.9509E-07	1.4060E-10	150	1500
220	C10H22	5-METHYLNONANE	46.011	6.3913E-01	1.2507E-04	-4.1575E-07	1.4602E-10	150	1500
221	C10H22O	1-DECANOL	15.733	8.9157E-01	-3.3219E-04	-8.6679E-08	6.1276E-11	200	1500
222	C10H22O	DI-n-PENTYL ETHER	-17.080	1.0765E+00	-7.2109E-04	2.5716E-07	-3.9483E-11	298	1500
223	C10H22O	ISODECANOL	-34.228	1.1729E+00	-8.9588E-04	3.7908E-07	-6.8013E-11	298	1500
224	C10H22O5	TETRAETHYLENE GLYCOL DIMETHYL ETHER	-62.043	1.4737E+00	-1.2136E-03	5.2774E-07	-9.7123E-11	298	1500
225	C10H22S	n-DECYL MERCAPTAN	70.441	6.2988E-01	1.4669E-04	-4.2347E-07	1.4459E-10	200	1500
226	C10H23N	n-DECYLAMINE	-9.825	1.0697E+00	-6.7989E-04	2.1931E-07	-2.9272E-11	298	1500
227	C11H10	1-METHYLNAPHTHALENE	-8.325	6.5561E-01	-2.3148E-04	-8.6605E-08	5.3577E-11	200	1500
228	C11H10	2-METHYLNAPHTHALENE	-0.899	6.1854E-01	-1.8095E-04	-1.1454E-07	5.9208E-11	200	1500
229	C11H14O2	n-BUTYL BENZOATE	-84.783	1.1780E+00	-9.7914E-04	4.2833E-07	-7.6038E-11	298	1500
230	C11H16	n-PENTYLBENZENE	-4.484	7.7970E-01	-2.7838E-04	-7.5740E-08	5.1215E-11	200	1500
231	C11H16O	p-tert-AMYLPHENOL	-71.475	1.2516E+00	-1.0881E-03	4.9607E-07	-9.3224E-11	298	1500
232	C11H20O2	2-ETHYLHEXYL ACRYLATE	-44.392	1.3753E+00	-1.2506E-03	6.2600E-07	-1.2931E-10	298	1500
233	C11H22	1-UNDECENE	132.612	2.4011E-01	8.5062E-04	-9.4540E-07	2.8339E-10	150	1500
234	C11H22O	1-UNDECANAL	2.102	1.0578E+00	-6.7455E-04	2.2287E-07	-3.1192E-11	298	1500
235	C11H24	n-UNDECANE	125.212	3.1401E-01	7.9137E-04	-9.1410E-07	2.7568E-10	150	1500
236	C11H24O	1-UNDECANOL	16.702	9.7755E-01	-3.6662E-04	-9.5146E-08	6.7752E-11	200	1500
237	C11H24S	UNDECYL MERCAPTAN	74.322	6.9712E-01	1.5160E-04	-4.6448E-07	1.6008E-10	200	1500
238	C12H8O	DIBENZOFURAN	-14.004	5.8793E-01	9.7079E-05	-4.4225E-07	1.6599E-10	100	1500
239	C12H9N	DIBENZOPYRROLE	-117.362	1.3214E+00	-1.3019E-03	6.4403E-07	-1.2737E-10	298	1500
240	C12H10	ACENAPHTHENE	-61.063	9.6388E-01	-7.2100E-04	2.6234E-07	-3.6857E-11	200	1500
241	C12H10	BIPHENYL	-29.153	7.6716E-01	-3.4341E-04	-3.7724E-08	4.6179E-11	200	1500
242	C12H10O	DIPHENYL ETHER	-118.442	1.2856E+00	-1.2190E-03	5.9127E-07	-1.1547E-10	298	1500
243	C12H11N	p-AMINODIPHENYL	-95.528	1.2611E+00	-1.1955E-03	5.8242E-07	-1.1477E-10	298	1500
244	C12H11N	DIPHENYLAMINE	-119.401	1.3060E+00	-1.2200E-03	5.8764E-07	-1.1447E-10	298	1500
245	C12H11N3	p-AMINOAZOBENZENE	-160.867	1.7547E+00	-1.9301E-03	1.0499E-06	-2.2321E-10	298	1500
246	C12H11N3	1,3-DIPHENYLTRIAZENE	-190.085	1.8079E+00	-1.9564E-03	1.0452E-06	-2.1809E-10	298	1500
247	C12H12	2,6-DIMETHYLNAPHTHALENE	-49.867	1.0029E+00	-7.9843E-04	3.3597E-07	-5.8987E-11	298	1500
248	C12H12	2,7-DIMETHYLNAPHTHALENE	-49.867	1.0029E+00	-7.9843E-04	3.3597E-07	-5.8987E-11	298	1500
249	C12H12	1-ETHYLNAPHTHALENE	-77.162	1.1312E+00	-9.8675E-04	4.5204E-07	-8.5024E-11	298	1500
250	C12H12N2	p-AMINODIPHENYLAMINE	-109.455	1.3879E+00	-1.3126E-03	6.3299E-07	-1.2318E-10	298	1500
251	C12H12N2	HYDRAZOBENZENE	-116.092	1.3797E+00	-1.3149E-03	6.4282E-07	-1.2675E-10	298	1500
252	C12H14	1,2,3-TRIMETHYLINDENE	-37.324	1.0980E+00	-9.2975E-04	4.1878E-07	-7.8898E-11	298	1500
253	C12H14O4	DIETHYL PHTHALATE	-122.210	1.4777E+00	-1.3850E-03	6.7906E-07	-1.3210E-10	298	1500
254	C12H16	CYCLOHEXYLBENZENE	-94.764	1.1349E+00	-6.8154E-04	1.4688E-07	2.5822E-12	298	1400
255	C12H18	m-DIISOPROPYLBENZENE	-70.177	1.2283E+00	-9.8495E-04	4.2208E-07	-7.6005E-11	298	1500
256	C12H18	p-DIISOPROPYLBENZENE	-70.177	1.2283E+00	-9.8495E-04	4.2208E-07	-7.6005E-11	298	1500
257	C12H18	n-HEXYLBENZENE	39.655	6.4328E-01	6.6681E-05	-3.5564E-07	1.2779E-10	200	1500
258	C12H20O4	DIBUTYL MALEATE	68.479	9.1396E-01	-4.0061E-04	1.5325E-08	2.1770E-11	298	1500
259	C12H22	BICYCLOHEXYL	-122.649	1.3647E+00	-7.9966E-04	1.8314E-07	-5.1919E-12	298	1500
260	C12H23N	DICYCLOHEXYLAMINE	-128.032	1.4622E+00	-8.6193E-04	1.8462E-07	3.6227E-13	298	1500
261	C12H24	1-DODECENE	83.102	6.2741E-01	2.2136E-04	-4.7938E-07	1.5890E-10	200	1500
262	C12H24O	1-DODECANAL	4.271	1.1290E+00	-6.7200E-04	1.8542E-07	-1.7582E-11	298	1500
263	C12H24O2	n-DODECANOIC ACID	-4.295	1.2373E+00	-8.2209E-04	2.7680E-07	-3.8871E-11	298	1500
264	C12H26	n-DODECANE	71.498	7.2559E-01	1.1553E-04	-4.1196E-07	1.4141E-10	200	1500
265	C12H26O	DI-n-HEXYL ETHER	-18.114	1.2587E+00	-8.1053E-04	2.6448E-07	-3.5458E-11	298	1500
266	C12H26O	1-DODECANOL	17.965	1.0602E+00	-3.9244E-04	-1.1142E-07	7.6380E-11	200	1500
267	C12H26O3	DIETHYLENE GLYCOL DI-n-BUTYL ETHER	-45.437	1.5002E+00	-1.1545E-03	4.8538E-07	-8.9144E-11	298	1500
268	C12H26S	n-DODECYL MERCAPTAN	-15.335	1.2989E+00	-9.1285E-04	3.6369E-07	-6.4587E-11	298	1500
269	C12H27BO3	TRI-n-BUTYL BORATE	---	---	---	---	---	--	--
270	C12H27N	DODECYLAMINE	-18.410	1.3048E+00	-8.9181E-04	3.3488E-07	-5.5494E-11	298	1500
271	C12H27N	TRI-n-BUTYLAMINE	-52.703	1.4429E+00	-1.0614E-03	4.2083E-07	-7.1662E-11	298	1500
272	C13H10	FLUORENE	-74.758	1.0187E+00	-7.1721E-04	2.2140E-07	-2.0280E-11	200	1500
273	C13H10O	BENZOPHENONE	-75.275	1.0612E+00	-7.8307E-04	2.7117E-07	-3.4873E-11	298	1500
274	C13H12	DIPHENYLMETHANE	-100.298	1.2250E+00	-1.0670E-03	4.8040E-07	-8.7845E-11	298	1600
275	C13H20	n-HEPTYLBENZENE	45.886	7.0113E-01	7.7233E-05	-3.9047E-07	1.3976E-10	200	1500
276	C13H26	1-TRIDECENE	88.663	6.8861E-01	2.2611E-04	-5.0981E-07	1.6963E-10	200	1500
277	C13H26O	1-TRIDECANAL	-1.839	1.2551E+00	-7.8737E-04	2.4389E-07	-2.9663E-11	298	1500
278	C13H26O2	n-BUTYL NONANOATE	-58.657	1.6081E+00	-1.3740E-03	6.5735E-07	-1.3319E-10	298	1500

$C_p = A + B\,T + C\,T^2 + D\,T^3 + E\,T^4$ (C_p - joule/g-mol K, T - K)

NO	FORMULA	NAME	A	B	C	D	E	TMIN	TMAX
279	C13H26O2	METHYL DODECANOATE	-28.448	1.4656E+00	-1.1419E-03	4.9828E-07	-9.3415E-11	298	1500
280	C13H28	n-TRIDECANE	110.400	5.3321E-01	7.3984E-04	-1.0212E-06	3.2423E-10	150	1500
281	C13H28O	1-TRIDECANOL	19.127	1.1452E+00	-4.2519E-04	-1.2106E-07	8.3188E-11	200	1500
282	C14H8O2	ANTHRAQUINONE	-77.119	1.2856E+00	-1.3749E-03	9.3187E-07	-3.0596E-10	298	900
283	C14H10	ANTHRACENE	-68.180	1.0788E+00	-8.1286E-04	2.9013E-07	-3.8196E-11	200	1500
284	C14H10	DIPHENYLACETYLENE	-69.864	1.0800E+00	-8.1462E-04	2.8054E-07	-3.3905E-11	298	1500
285	C14H10	PHENANTHRENE	-73.218	1.1192E+00	-8.9679E-04	3.5695E-07	-5.6466E-11	200	1500
286	C14H12	cis-STILBENE	-96.782	1.2486E+00	-1.0880E-03	5.0166E-07	-9.5052E-11	298	1500
287	C14H12	trans-STILBENE	-68.882	1.1174E+00	-8.3787E-04	3.0198E-07	-4.2209E-11	298	1500
288	C14H12O2	BENZYL BENZOATE	-137.070	1.4041E+00	-1.1419E-03	4.2281E-07	-4.5129E-11	298	1200
289	C14H14	1,1-DIPHENYLETHANE	-101.538	1.3208E+00	-1.1248E-03	4.9731E-07	-8.9846E-11	298	1600
290	C14H14	1,2-DIPHENYLETHANE	-101.104	1.3200E+00	-1.1240E-03	4.9709E-07	-8.9901E-11	298	1600
291	C14H14O	DIBENZYL ETHER	-133.169	1.4371E+00	-1.2020E-03	5.1612E-07	-9.1168E-11	298	1500
292	C14H16	1-n-BUTYLNAPHTHALENE	71.101	4.0054E-01	7.3214E-04	-9.7479E-07	3.1420E-10	100	1500
293	C14H22	n-OCTYLBENZENE	51.588	7.6266E-01	8.0566E-05	-4.2003E-07	1.5047E-10	200	1500
294	C14H22O	p-tert-OCTYLPHENOL	-99.971	1.6764E+00	-1.4559E-03	6.5521E-07	-1.2088E-10	298	1500
295	C14H28	1-TETRADECENE	167.903	3.1544E-01	1.0739E-03	-1.2004E-06	3.6046E-10	150	1500
296	C14H28O2	n-TETRADECANOIC ACID	-47.091	1.5789E+00	-1.1521E-03	4.4718E-07	-7.3810E-11	298	1500
297	C14H30	n-TETRADECANE	115.502	6.0882E-01	6.8043E-04	-9.7091E-07	3.0756E-10	150	1500
298	C14H30O	1-TETRADECANOL	20.531	1.2268E+00	-4.4901E-04	-1.3852E-07	9.2055E-11	200	1500
299	C14H31N	TETRADECYLAMINE	-23.409	1.5091E+00	-1.0193E-03	3.6745E-07	-5.6794E-11	298	1500
300	C15H10N2O2	DIPHENYLMETHANE-4,4'-DIISOCYANATE	-40.814	1.1664E+00	-8.2318E-04	2.6180E-07	-2.8364E-11	298	1500
301	C15H16O	p-CUMYLPHENOL	-105.972	1.5282E+00	-1.3205E-03	5.8321E-07	-1.0494E-10	298	1500
302	C15H16O2	BISPHENOL A	-106.990	1.6818E+00	-1.6100E-03	7.9103E-07	-1.5526E-10	298	1600
303	C15H24	n-NONYLBENZENE	0.378	1.1149E+00	-3.9485E-04	-1.2822E-07	8.2222E-11	200	1500
304	C15H24O	2,6-DI-tert-BUTYL-p-CRESOL	-85.106	1.6932E+00	-1.3931E-03	5.9127E-07	-1.0339E-10	298	1500
305	C15H24O	NONYLPHENOL	-51.387	1.5081E+00	-1.1306E-03	4.4257E-07	-7.2709E-11	298	1500
306	C15H30	1-PENTADECENE	26.049	1.1942E+00	-3.8640E-04	-1.8619E-07	1.0451E-10	200	1500
307	C15H30O2	PENTADECANOIC ACID	-12.682	1.5569E+00	-1.0581E-03	3.7408E-07	-5.6293E-11	298	1500
308	C15H32	n-PENTADECANE	124.647	6.2706E-01	8.3164E-04	-1.1689E-06	3.7326E-10	150	1500
309	C16H10	FLUORANTHENE	-112.910	1.4495E+00	-1.3602E-03	6.4245E-07	-1.2194E-10	298	1500
310	C16H10	PYRENE	27.191	5.8885E-01	2.4989E-04	-5.7314E-07	2.0114E-10	150	1500
311	C16H12	1-PHENYLNAPHTHALENE	-114.610	1.4322E+00	-1.2669E-03	5.7235E-07	-1.0505E-10	298	1500
312	C16H20	1-n-HEXYLNAPHTHALENE	-82.067	1.5218E+00	-1.2290E-03	5.2212E-07	-9.1550E-11	298	1500
313	C16H22O4	DIBUTYL PHTHALATE	148.647	-3.1458E-01	4.5159E-03	-6.5996E-06	3.0370E-09	298	800
314	C16H26	n-DECYLBENZENE	65.790	8.6789E-01	1.2244E-04	-5.0606E-07	1.7890E-10	200	1500
315	C16H32	n-DECYLCYCLOHEXANE	157.247	4.0618E-01	1.3486E-03	-1.5340E-06	4.6479E-10	150	1500
316	C16H32	1-HEXADECENE	108.689	8.5437E-01	2.7357E-04	-6.2732E-07	2.0929E-10	200	1500
317	C16H32O2	n-HEXADECANOIC ACID	-54.487	1.8046E+00	-1.3388E-03	5.3671E-07	-9.2028E-11	298	1500
318	C16H34	n-HEXADECANE	131.750	6.7397E-01	8.7770E-04	-1.2430E-06	3.9785E-10	150	1500
319	C16H34O	DI-n-OCTYL ETHER	-33.322	1.7059E+00	-1.1626E-03	4.2114E-07	-6.4955E-11	298	1500
320	C16H34O	1-HEXADECANOL	119.789	8.1674E-01	6.2364E-04	-1.0540E-06	3.4977E-10	150	1500
321	C17H28	n-UNDECYLBENZENE	2.711	1.2830E+00	-4.5442E-04	-1.5326E-07	9.7372E-11	200	1500
322	C17H34	1-HEPTADECENE	125.132	7.9164E-01	6.6154E-04	-1.0780E-06	3.5594E-10	150	1500
323	C17H36	n-HEPTADECANE	111.903	9.5987E-01	2.7901E-04	-6.7520E-07	2.2545E-10	200	1500
324	C17H36O	1-HEPTADECANOL	127.444	8.7086E-01	6.4059E-04	-1.0987E-06	3.6628E-10	150	1500
325	C18H12	CHRYSENE	-41.414	1.1172E+00	-5.6061E-04	1.7203E-09	5.1921E-11	200	1500
326	C18H14	m-TERPHENYL	-159.334	1.8173E+00	-1.7948E-03	9.0423E-07	-1.7969E-10	298	1600
327	C18H14	o-TERPHENYL	-159.334	1.8173E+00	-1.7948E-03	9.0423E-07	-1.7969E-10	298	1600
328	C18H14	p-TERPHENYL	-159.334	1.8173E+00	-1.7948E-03	9.0423E-07	-1.7969E-10	298	1600
329	C18H15P	TRIPHENYLPHOSPHINE	-140.077	1.8099E+00	-1.7088E-03	8.3604E-07	-1.6512E-10	298	1500
330	C18H15O4P	TRIPHENYL PHOSPHATE	---	---	---	---	---	--	--
331	C18H16N2	N,N'-DIPHENYL-p-PHENYLENEDIAMINE	-188.536	2.0474E+00	-1.9559E-03	9.5063E-07	-1.8600E-10	298	1500
332	C18H22	2,3-DIMETHYL-2,3-DIPHENYLBUTANE	-159.612	1.9863E+00	-1.7695E-03	8.1753E-07	-1.5467E-10	298	1500
333	C18H22O2	DICUMYL PEROXIDE	-76.744	1.6944E+00	-1.2744E-03	4.7912E-07	-7.3317E-11	298	1500
334	C18H30	n-DODECYLBENZENE	106.695	7.7941E-01	5.8463E-04	-9.4162E-07	3.0397E-10	150	1500
335	C18H32O2	LINOLEIC ACID	-113.518	2.1932E+00	-1.9690E-03	9.5258E-07	-1.7989E-10	298	1500
336	C18H34O2	OLEIC ACID	-55.663	1.9919E+00	-1.5562E-03	6.7067E-07	-1.2336E-10	298	1500
337	C18H34O4	DIBUTYL SEBACATE	-64.966	2.2026E+00	-1.8844E-03	8.8961E-07	-1.7701E-10	298	1500
338	C18H34O4	DIHEXYL ADIPATE	-64.614	2.0235E+00	-1.8000E-03	8.8573E-07	-1.8193E-10	298	1500
339	C18H36	1-OCTADECENE	216.021	4.1046E-01	1.3808E-03	-1.5473E-06	4.6513E-10	150	1500
340	C18H36O2	STEARIC ACID	7.515	1.6996E+00	-9.2847E-04	1.7563E-07	3.6437E-12	298	1200
341	C18H38	n-OCTADECANE	124.715	9.8653E-01	3.4273E-04	-7.4838E-07	2.4804E-10	200	1500
342	C18H38O	DINONYL ETHER	-39.993	1.9149E+00	-1.2953E-03	4.5896E-07	-6.9698E-11	298	1500
343	C18H38O	1-OCTADECANOL	129.533	9.2997E-01	6.6025E-04	-1.1313E-06	3.7237E-10	150	1500
344	C19H26	1-n-NONYLNAPHTHALENE	-76.861	1.7404E+00	-1.2853E-03	4.9048E-07	-7.7646E-11	298	1500
345	C19H32	n-TRIDECYLBENZENE	86.726	1.0288E+00	1.7917E-04	-6.3099E-07	2.2067E-10	200	1500
346	C19H36O2	METHYL OLEATE	-44.058	2.0299E+00	-1.5136E-03	6.1226E-07	-1.0656E-10	298	1500
347	C19H38	1-NONADECENE	69.594	1.2608E+00	3.8456E-06	-6.0097E-07	2.2323E-10	200	1500
348	C19H38O2	NONADECANOIC ACID	-23.711	1.9781E+00	-1.3539E-03	4.8185E-07	-7.2339E-11	298	1500
349	C19H40	n-NONADECANE	132.530	1.0358E+00	3.6926E-04	-7.9581E-07	2.6362E-10	200	1500
350	C20H16	TRIPHENYLETHYLENE	-122.663	1.7649E+00	-1.5644E-03	7.2308E-07	-1.3678E-10	298	1500

NO	FORMULA	NAME	$C_P = A + B\,T + C\,T^2 + D\,T^3 + E\,T^4$ (A	B	C	D	E	TMIN	TMAX
351	C20H28	1-n-DECYLNAPHTHALENE	-82.955	1.8664E+00	-1.4003E-03	5.4871E-07	-8.9673E-11	298	1500
352	C20H3002	ABIETIC ACID	-260.137	2.7296E+00	-2.3498E-03	1.0242E-06	-1.8203E-10	298	1500
353	C20H31N	DEHYDROABIETYLAMINE	-127.428	2.3347E+00	-2.0102E-03	9.0944E-07	-1.7163E-10	298	1200
354	C20H40	1-EICOSENE	125.107	1.1243E+00	2.5851E-04	-7.3027E-07	2.4754E-10	200	1500
355	C20H42	n-EICOSANE	137.730	1.0992E+00	3.6839E-04	-8.2058E-07	2.7259E-10	200	1500
356	C20H420	1-EICOSANOL	149.479	9.8474E-01	8.2856E-04	-1.3392E-06	4.3815E-10	150	1500
357	C21H2104P	TRI-o-CRESYL PHOSPHATE	---	---	---	---	---	--	--
358	C22H4402	n-BUTYL STEARATE	-69.046	2.5211E+00	-2.0966E-03	1.0835E-06	-2.7531E-10	298	1200
359	C24H3804	DIISOOCTYL PHTHALATE	-87.607	2.2843E+00	-1.3309E-03	2.5129E-07	1.4926E-11	298	1500
360	C24H3804	DIOCTYL PHTHALATE	-82.524	2.2568E+00	-1.2839E-03	2.1577E-07	2.8112E-11	298	1100
361	C24H420	DINONYLPHENOL	-21.466	2.1296E+00	-1.0229E-03	-8.3690E-08	1.5876E-10	298	1000
362	C26H20	TETRAPHENYLETHYLENE	-149.970	2.2370E+00	-1.9635E-03	8.9829E-07	-1.6846E-10	298	1500
363	C28H4604	DIISODECYL PHTHALATE	-128.947	2.9258E+00	-2.1855E-03	9.4298E-07	-2.1374E-10	298	1200

(C_P - joule/g-mol K, T - K)

Appendix F

COMPOUND LIST BY FORMULA

Appendix G

COMPOUND LIST BY NAME

Appendix H

Computer Program for Thermodynamic Properties

A computer program for calculation of thermodynamic properties using the Peng-Robinson equation of state is available for a nominal fee (Carl L. Yaws, Box 10053, Lamar University, Beaumont, TX 77710, phone/FAX 409-880-8787). The computer program is executable and complete with data files. The program calculates thermodynamic properties at pressures and temperatures that are input by the user. Representative results are shown below:

COMPOUND: 841 C8H18 n-OCTANE

reference state: datum of ideal gas @ 77 F (25 C)

P psia	T F	Z	V ft^3/lb	H BTU/lb	S BTU/lb F
500.0	0.00	0.266	0.023	-188.42	-0.292
500.0	100.00	0.228	0.024	-139.01	-0.195
500.0	200.00	0.204	0.025	-83.69	-0.104
500.0	300.00	0.192	0.027	-22.19	-0.018
500.0	400.00	0.190	0.031	46.12	0.067
500.0	500.00	0.206	0.037	123.11	0.151
500.0	1000.00	0.892	0.245	566.92	0.527
3000.0	0.00	1.573	0.023	-179.50	-0.296
3000.0	100.00	1.336	0.023	-130.64	-0.200
3000.0	200.00	1.181	0.024	-76.27	-0.111
3000.0	300.00	1.077	0.026	-16.44	-0.026
3000.0	400.00	1.011	0.027	48.72	0.054
3000.0	500.00	0.974	0.029	118.99	0.131
3000.0	1000.00	1.051	0.048	530.51	0.474
10000.0	0.00	5.132	0.022	-153.76	-0.303
10000.0	100.00	4.306	0.023	-105.62	-0.208
10000.0	200.00	3.741	0.023	-52.27	-0.121
10000.0	300.00	3.336	0.024	6.18	-0.038
10000.0	400.00	3.034	0.025	69.52	0.040
10000.0	500.00	2.804	0.025	137.49	0.115