

LIBRARY OF PHYSICO-CHEMICAL PROPERTY DATA

Handbook of Thermodynamic Diagrams



Volume 2

Organic
Compounds
C₅ to C₇

Carl L. Yaws

LIBRARY OF PHYSICO-CHEMICAL PROPERTY DATA

Handbook of Thermodynamic Diagrams



Volume 2

Organic
Compounds
C₅ to C₇

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LIBRARY OF PHYSICO-CHEMICAL PROPERTY DATA

Handbook of Thermodynamic Diagrams



Volume 2

Organic
Compounds
C₅ to C₇

Carl L. Yaws



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Handbook of Thermodynamic Diagrams, Volume 2

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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.

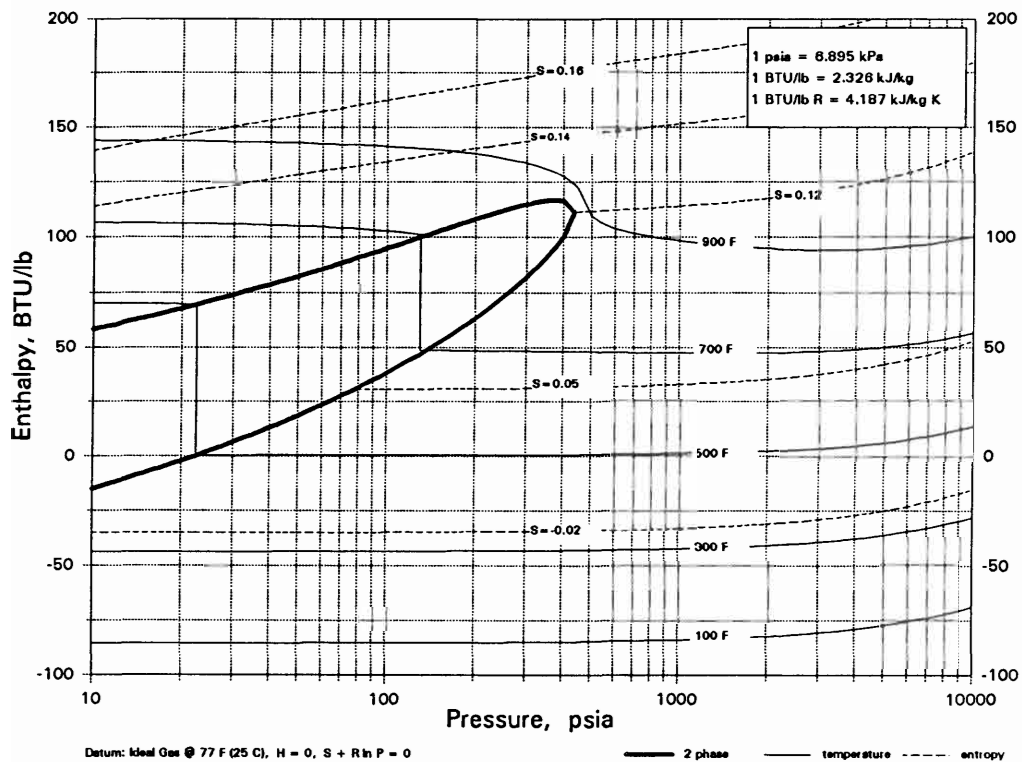
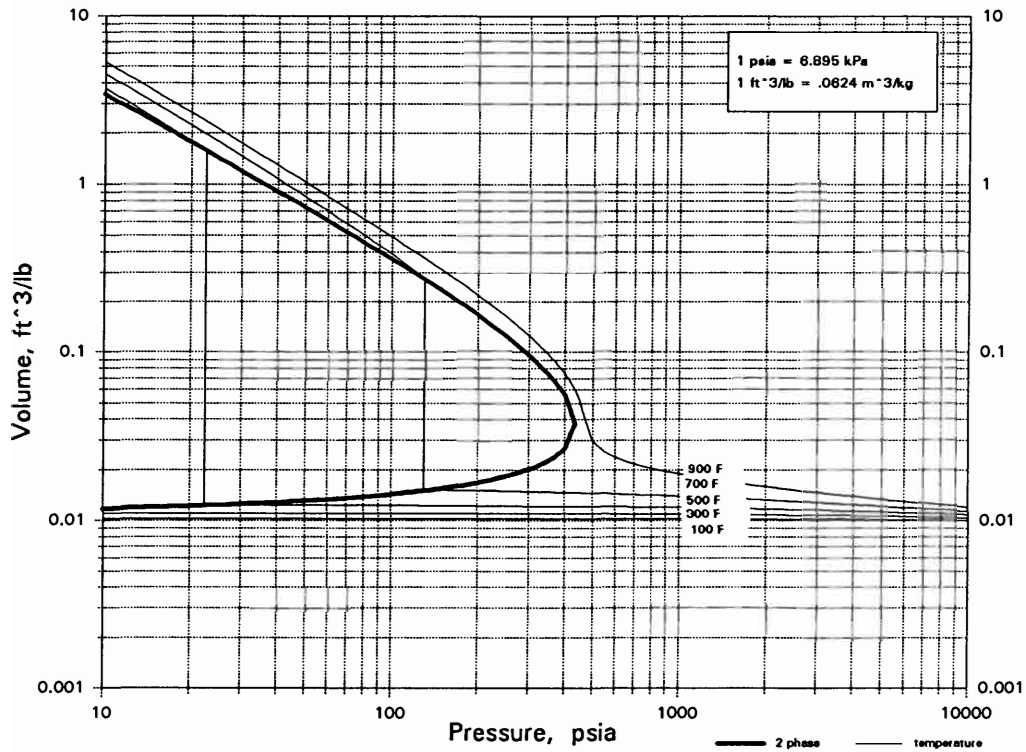
For the graphs, some of the compounds may undergo thermal decomposition (reaction) at the higher temperatures. For such cases of thermal decomposition, the graphs are useful for ascertaining property values of the pure compound which is contained in the reaction mixture. Chemistry handbooks and DIPPR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

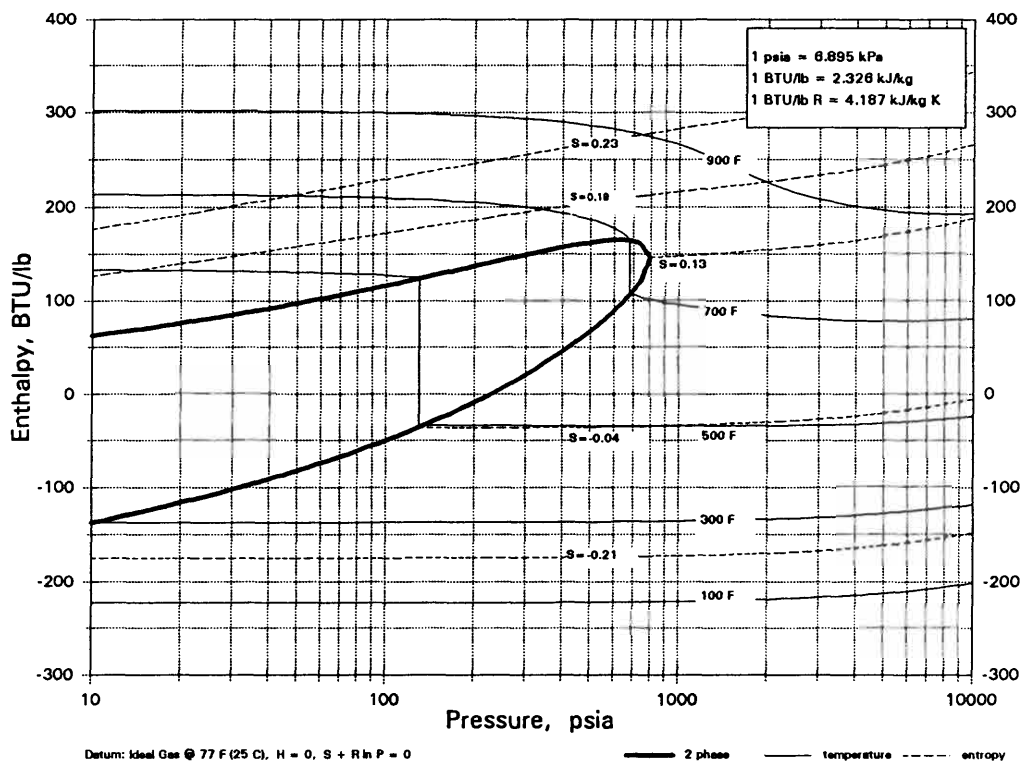
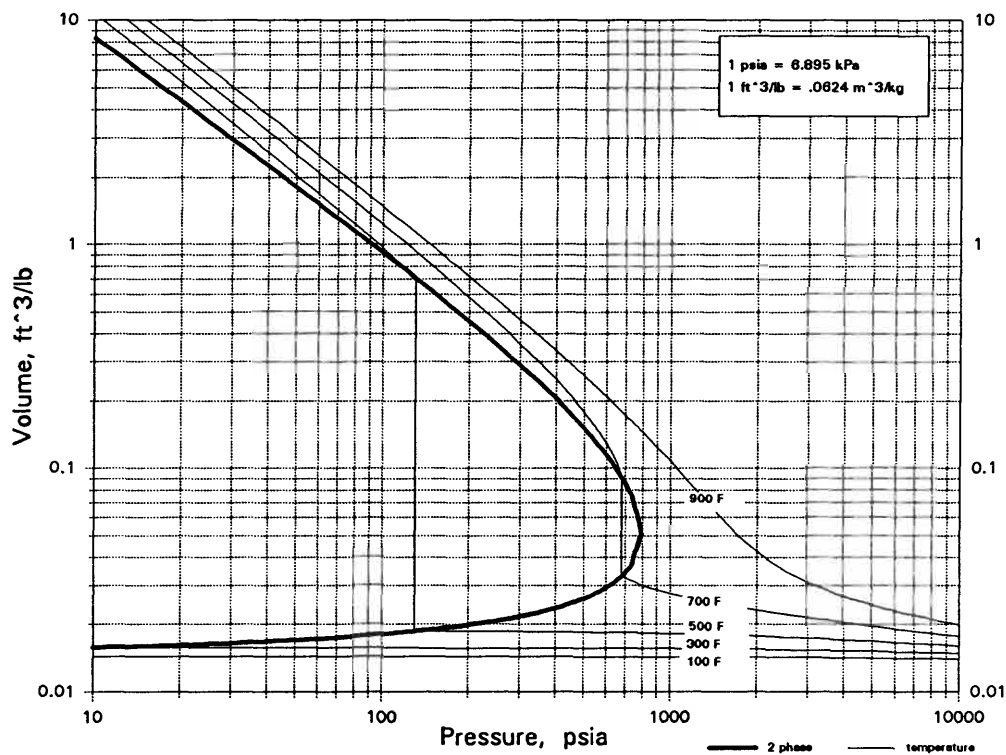
An executable computer program, complete with data files, is available for calculation of thermodynamic properties. For information on the program, contact Carl L. Yaws, Ph.D., P. O. Box 10053, Beaumont, Texas 77710, phone/fax (409) 880-8787.

C5Cl6

HEXACHLOROCYCLOPENTADIENE

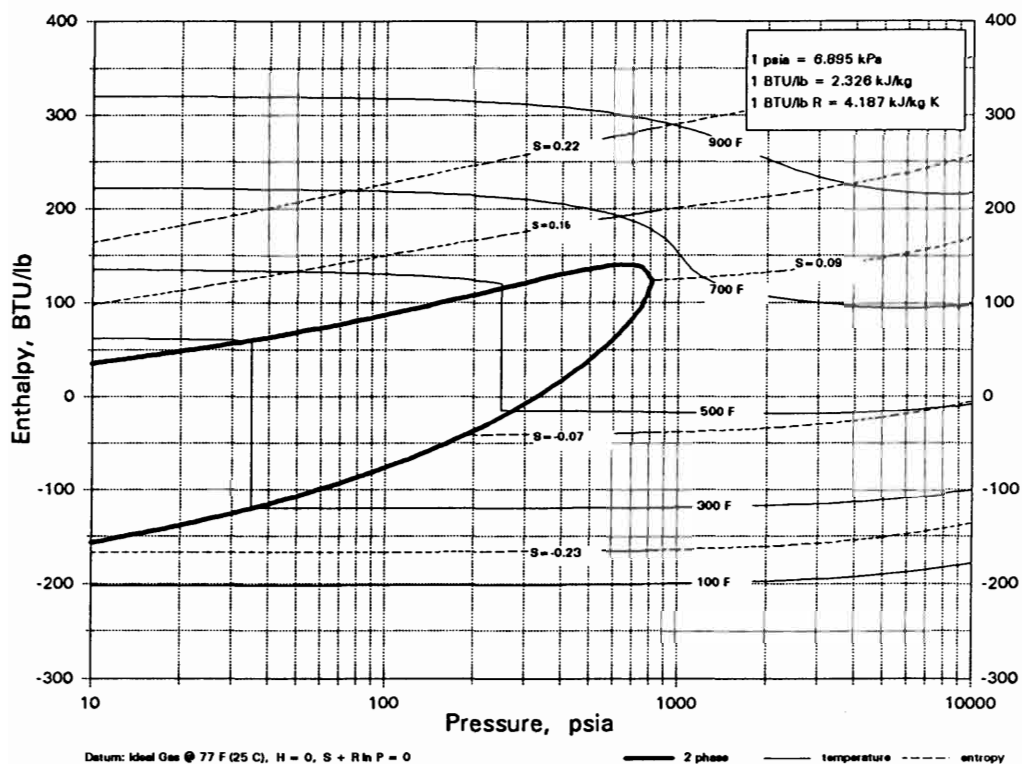
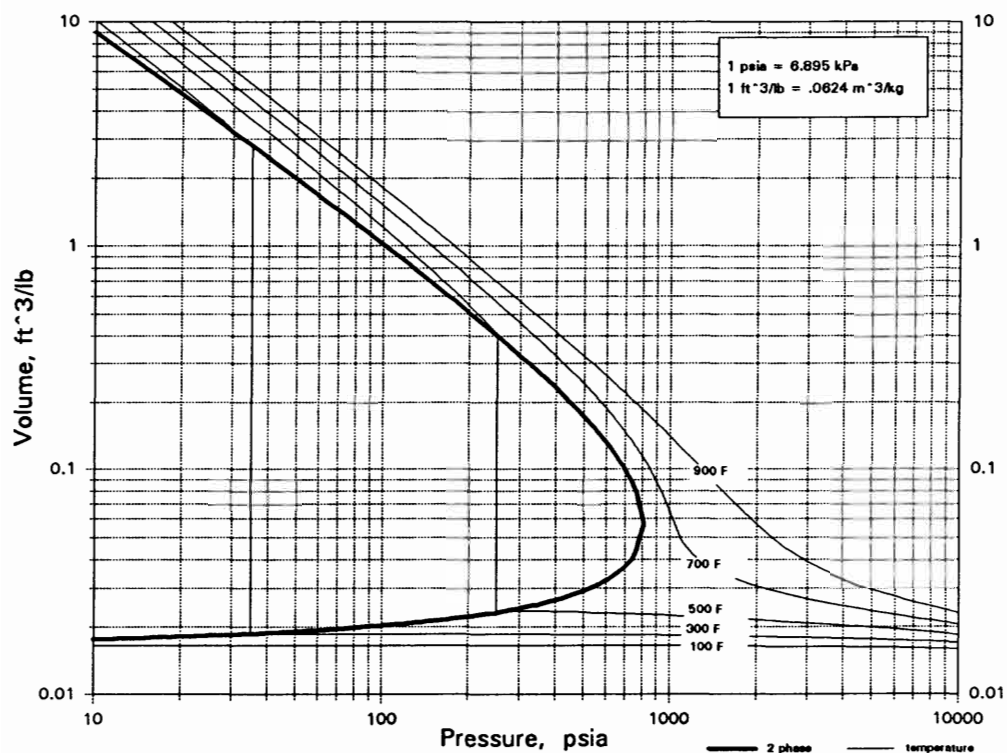


C5H4O2
FURFURAL



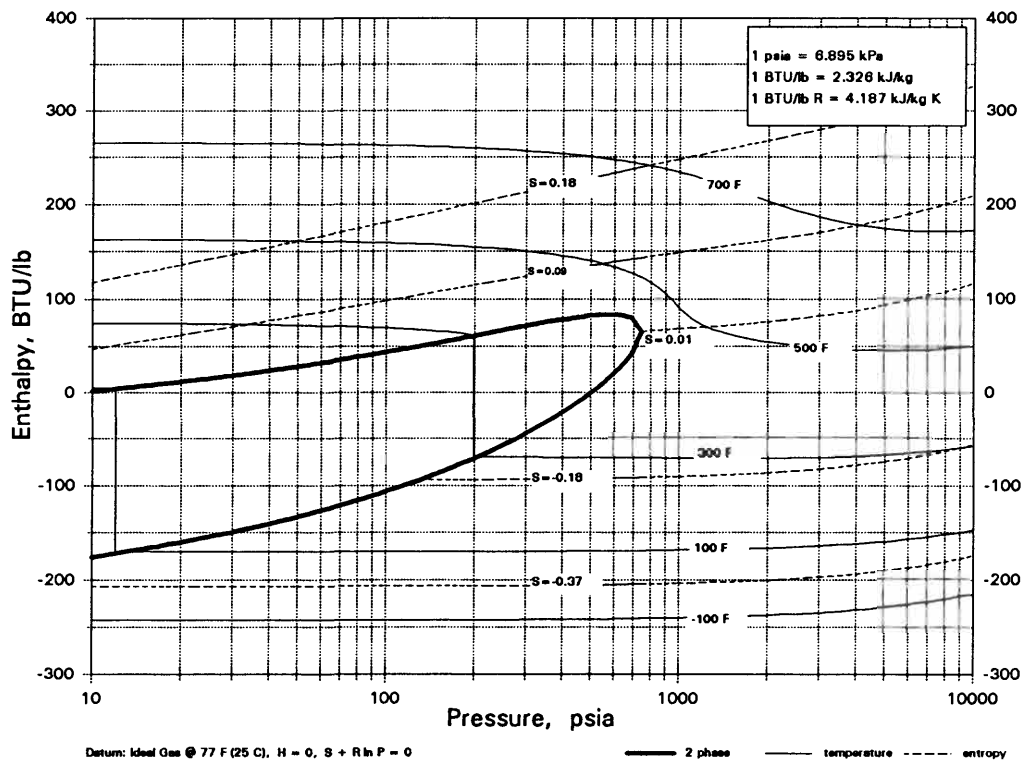
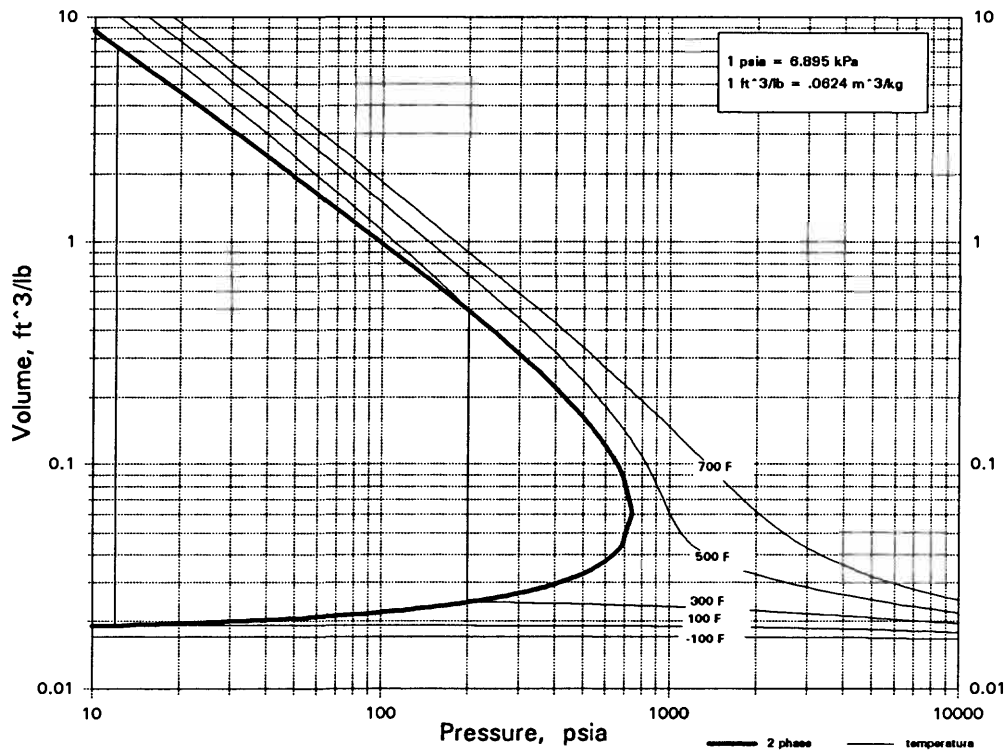
C5H5N

PYRIDINE



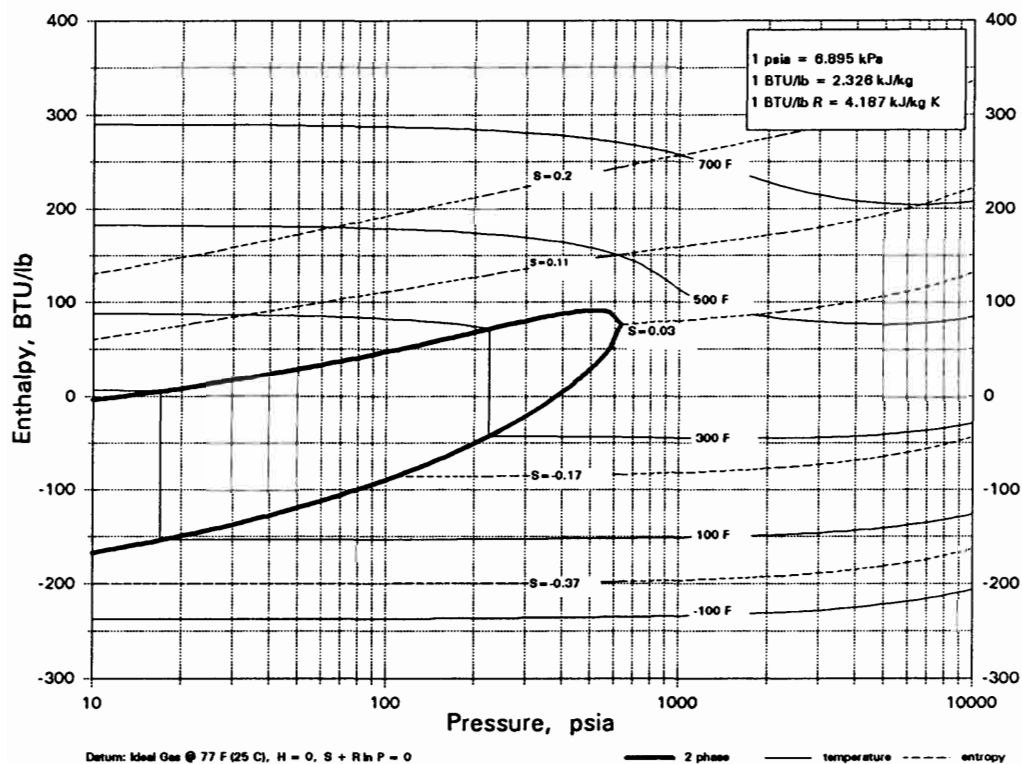
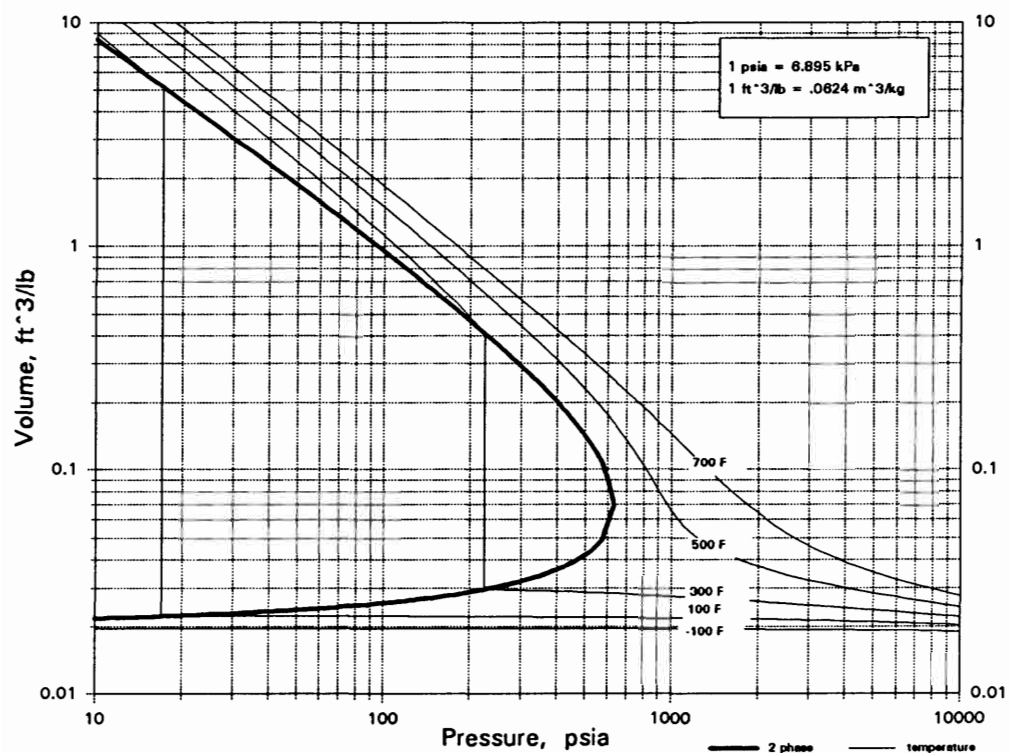
C5H6

CYCLOPENTADIENE



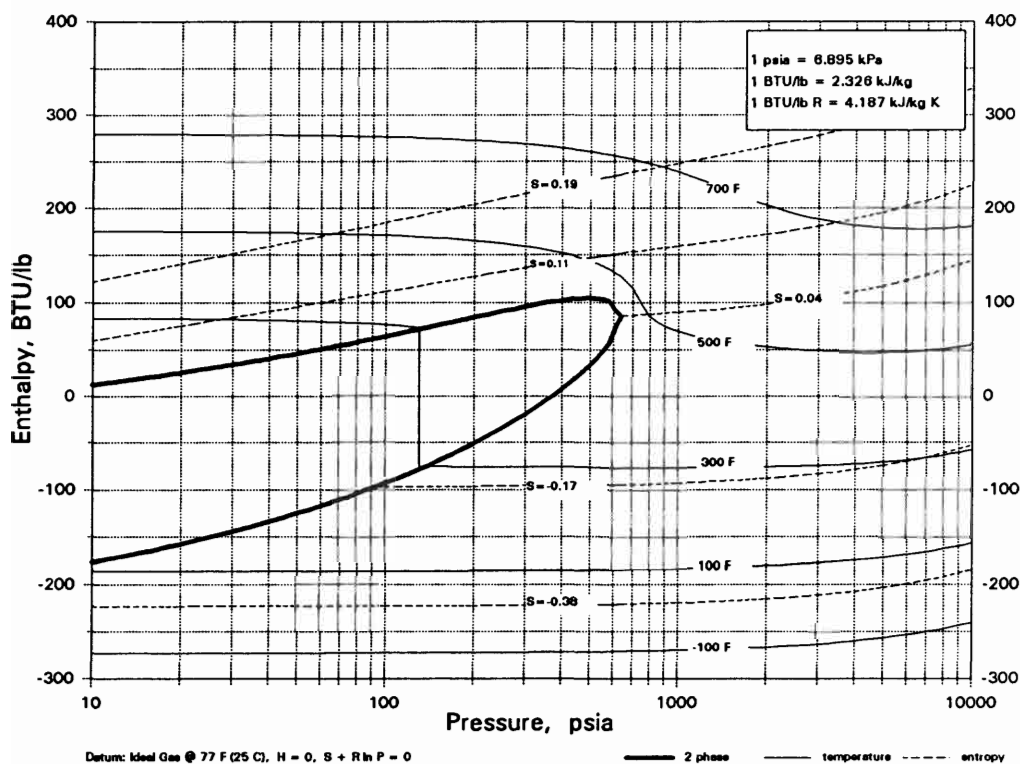
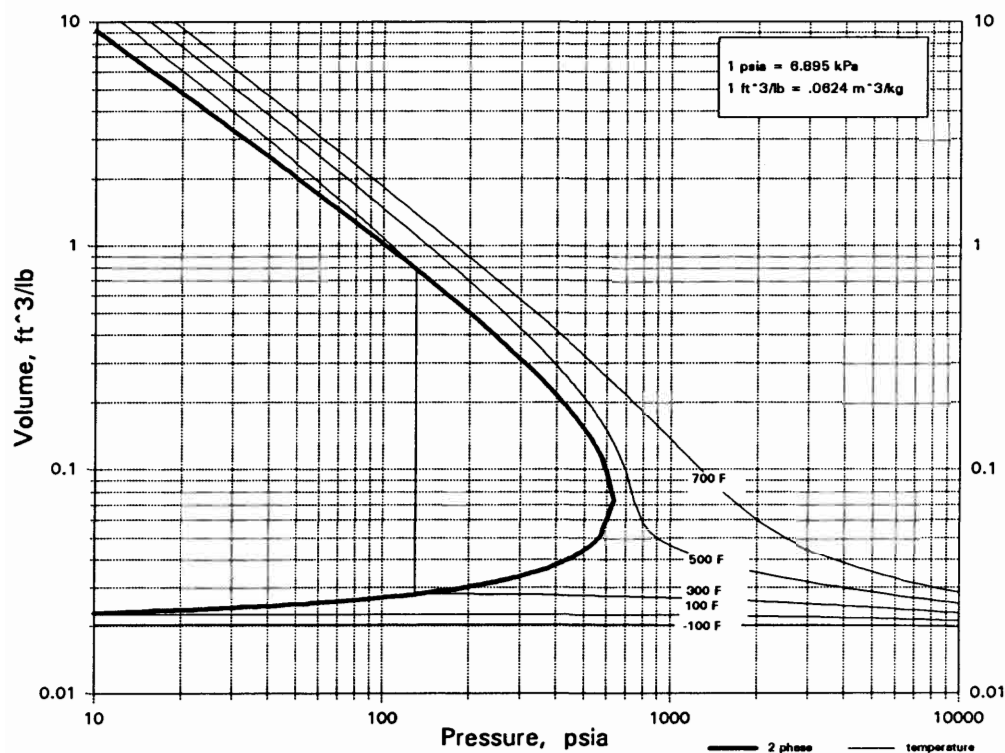
C5H6

2-METHYL-1-BUTENE-3-YNE



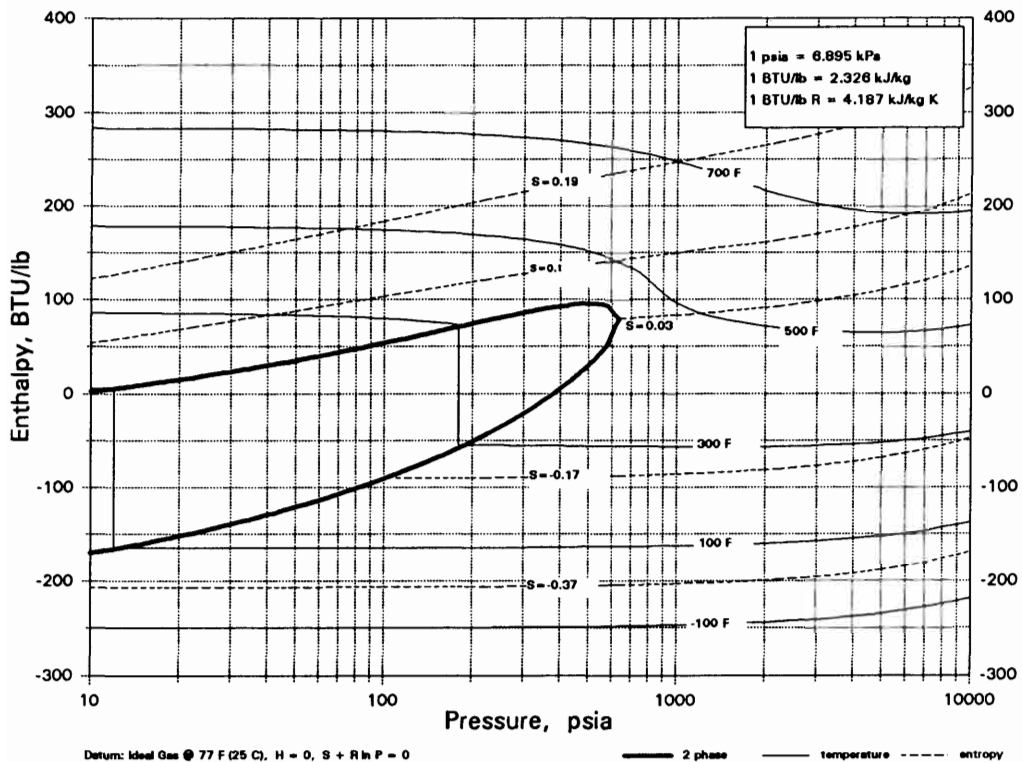
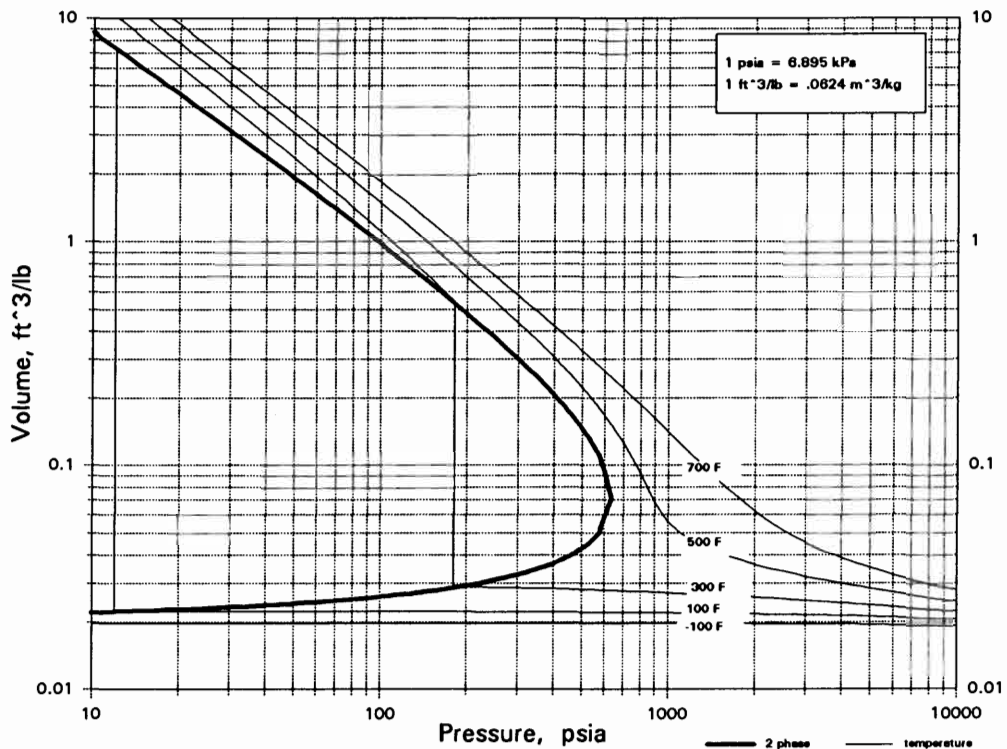
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1-PENTENE-3-YNE



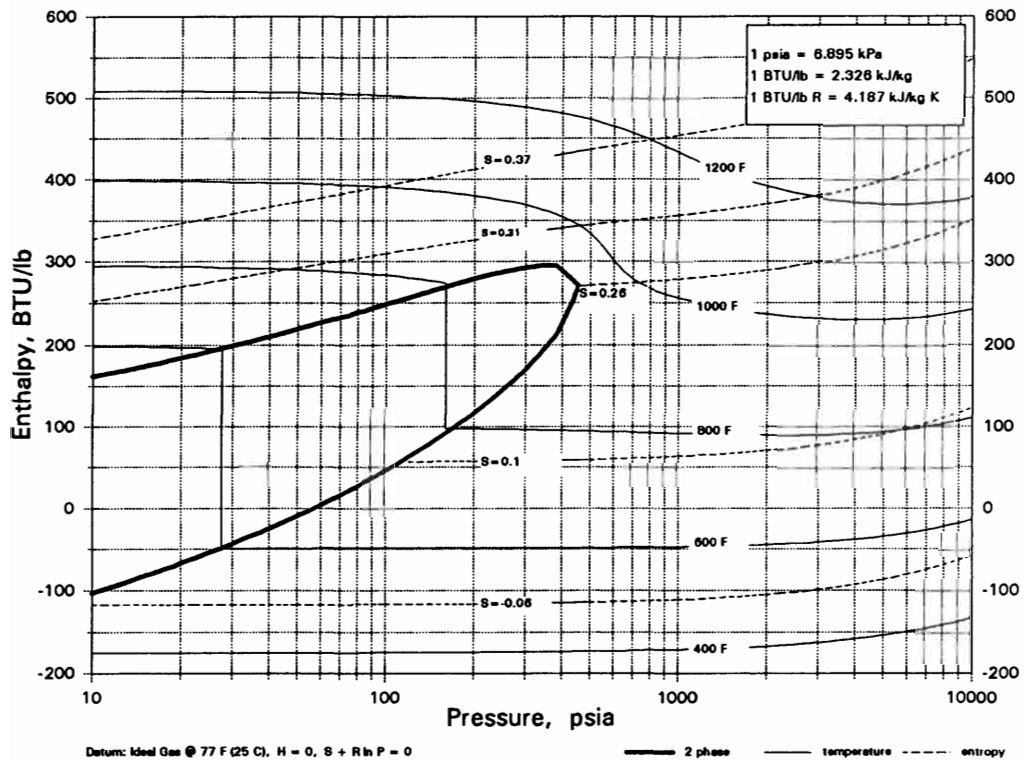
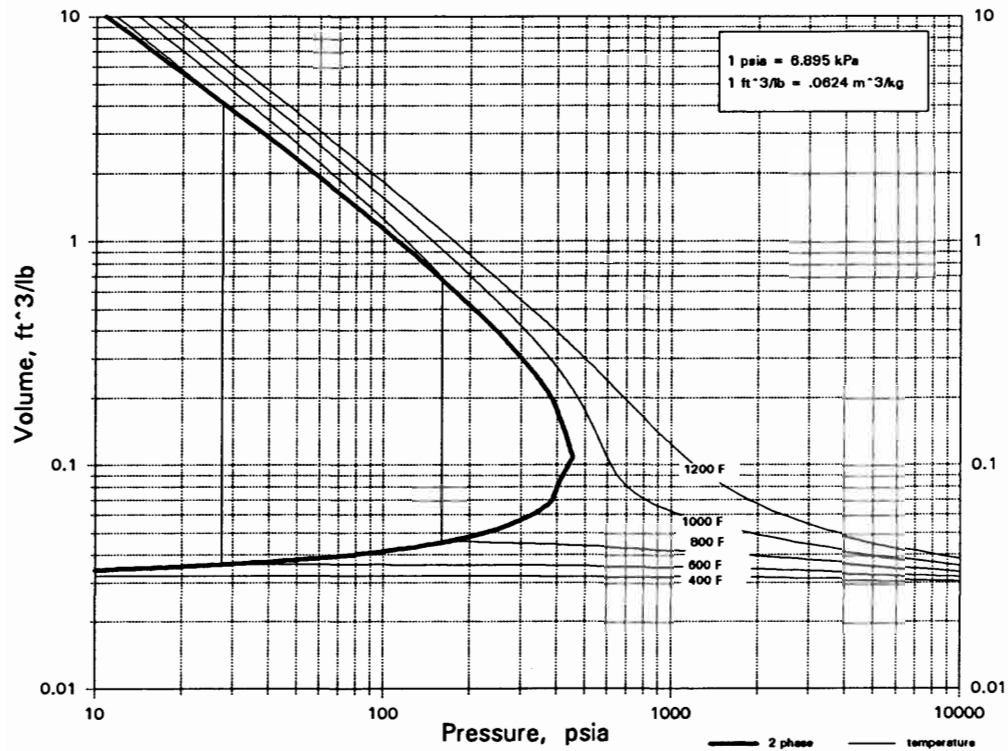
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1-PENTENE-4-YNE



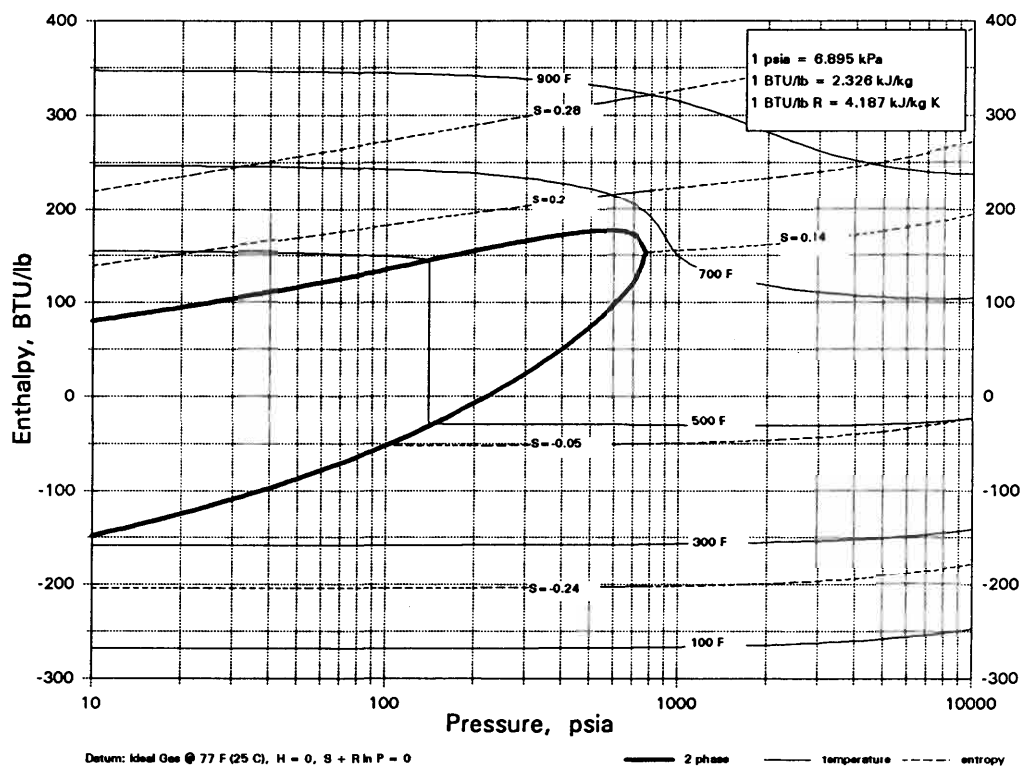
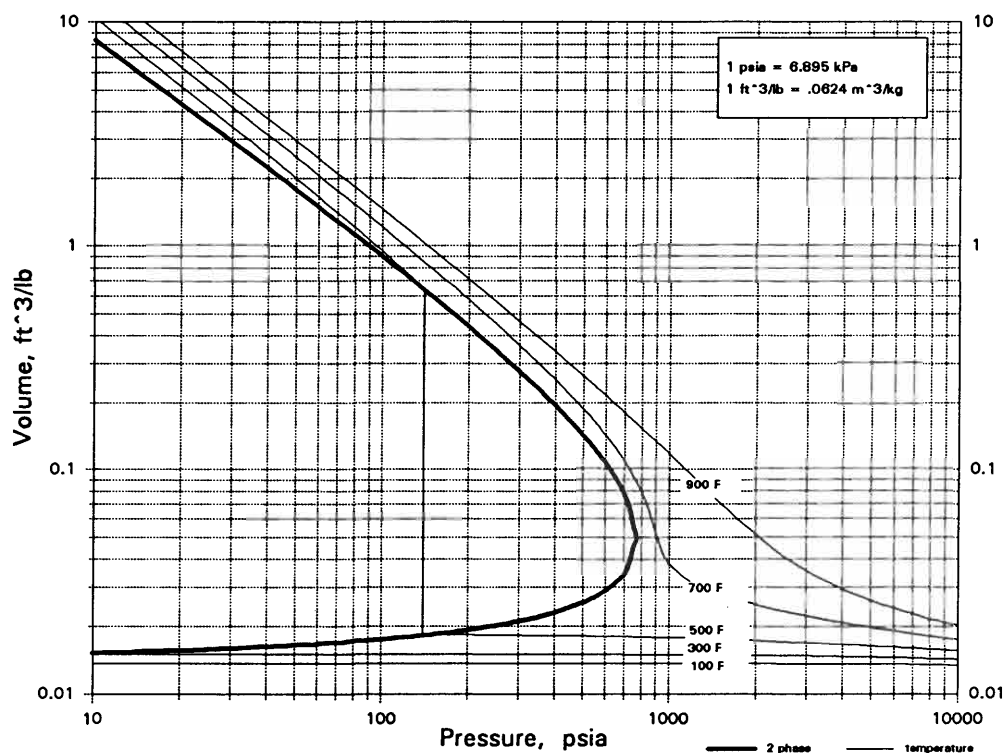
C5H6N2

GLUTARONITRILE

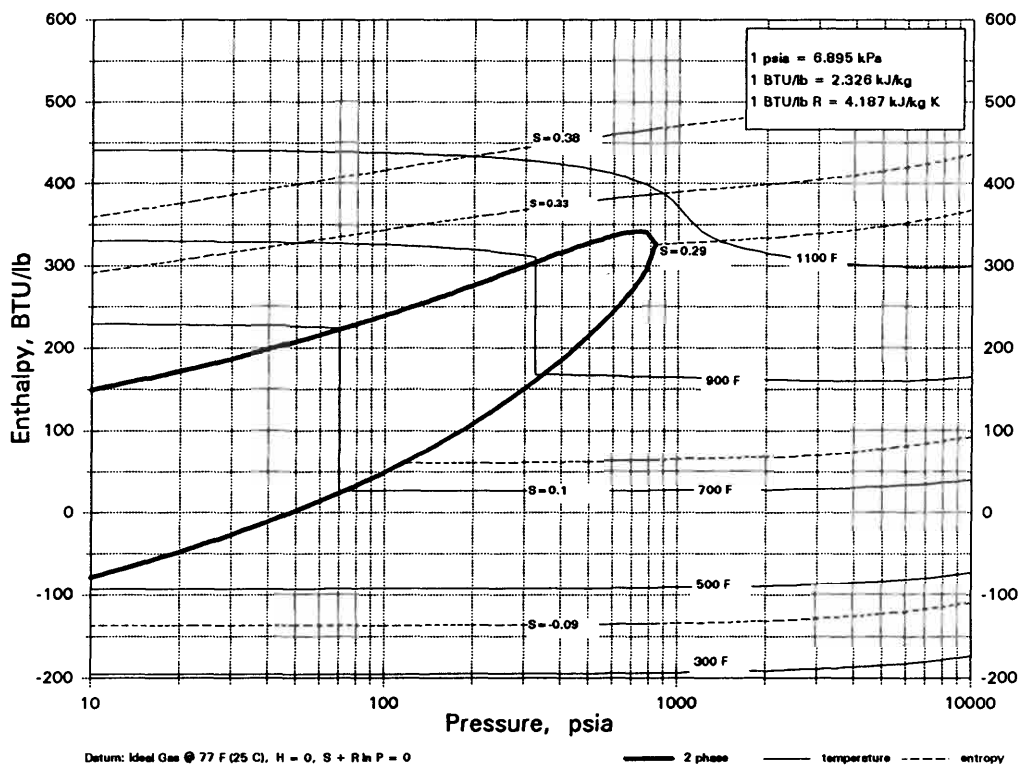
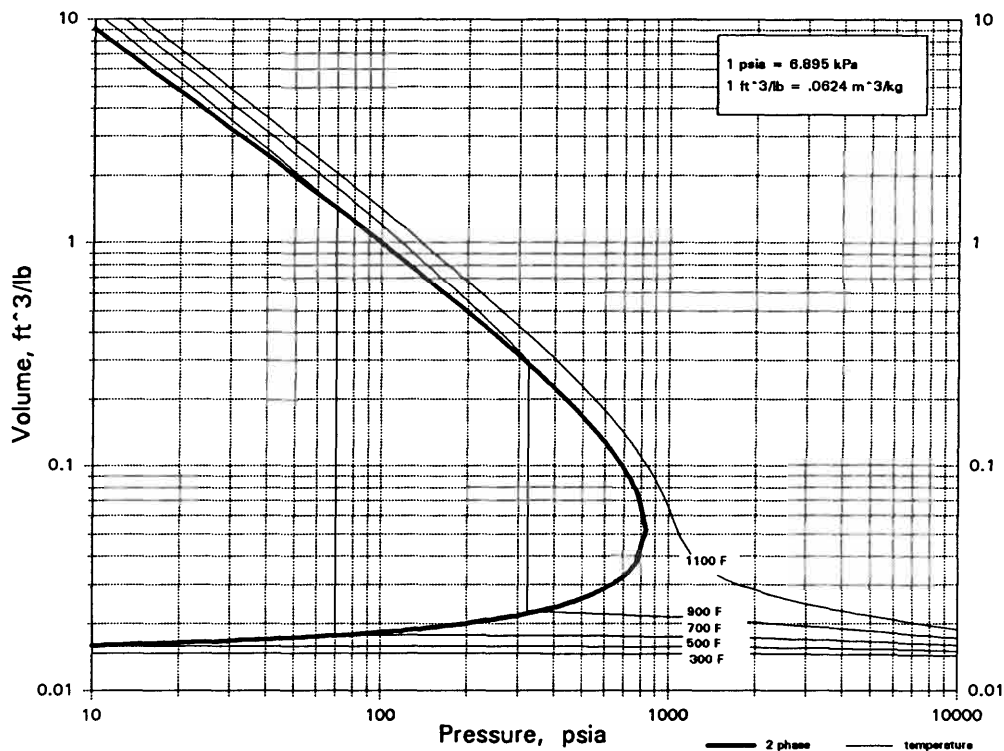


C5H6O2

FURFURYL ALCOHOL

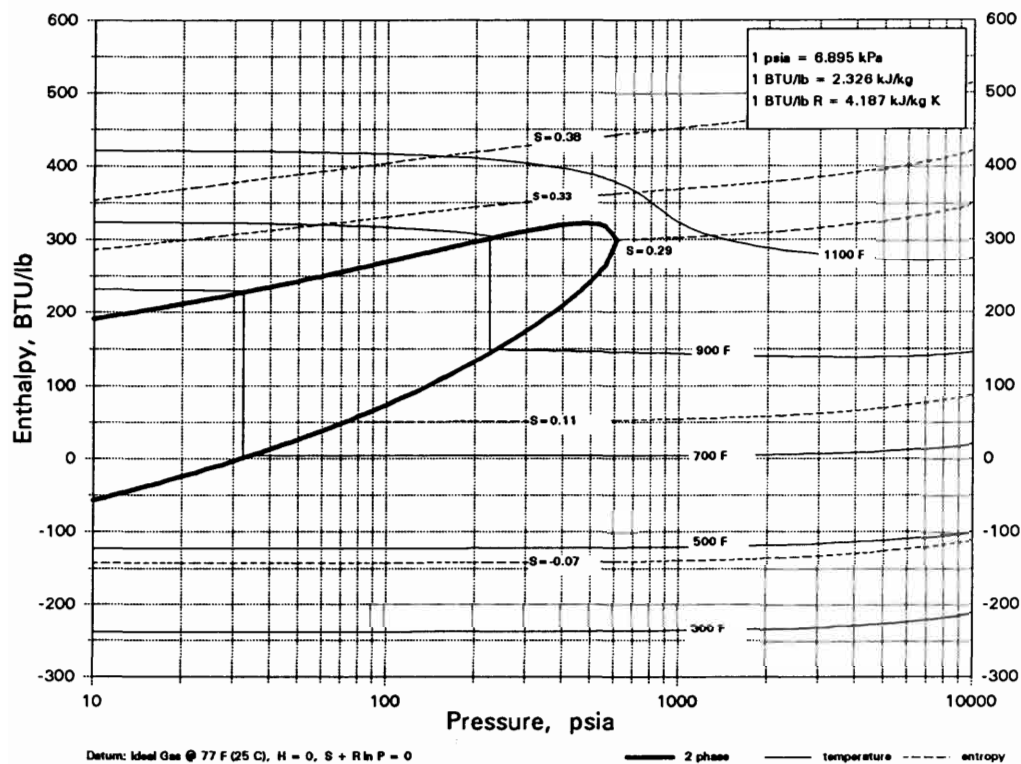
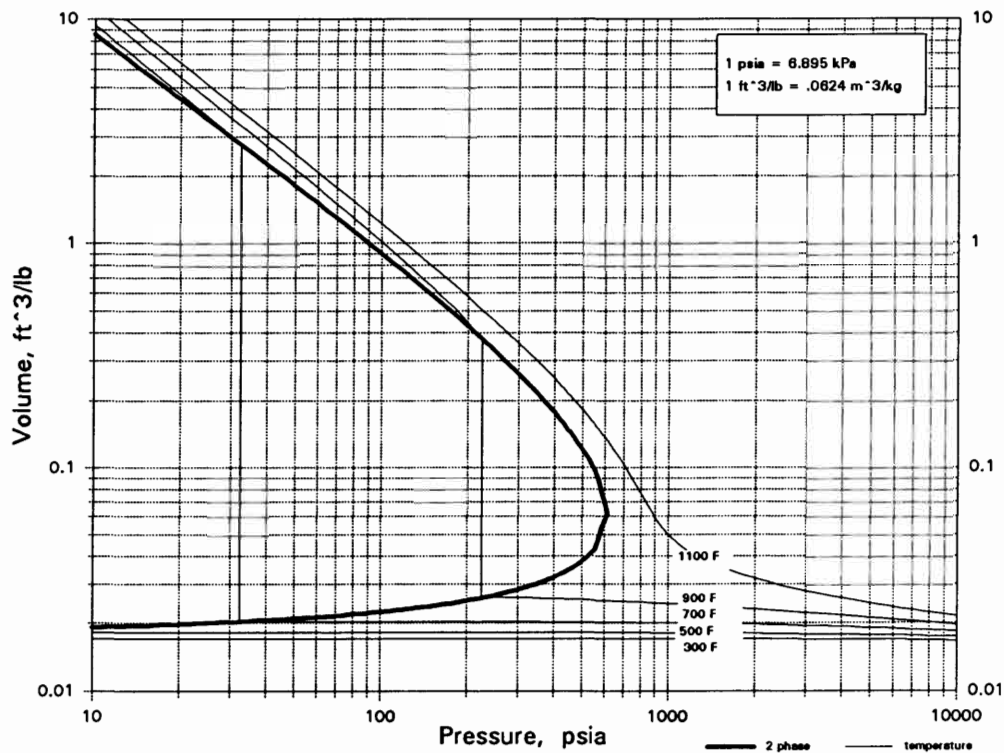


C5H6O3
GLUTARIC ANHYDRIDE



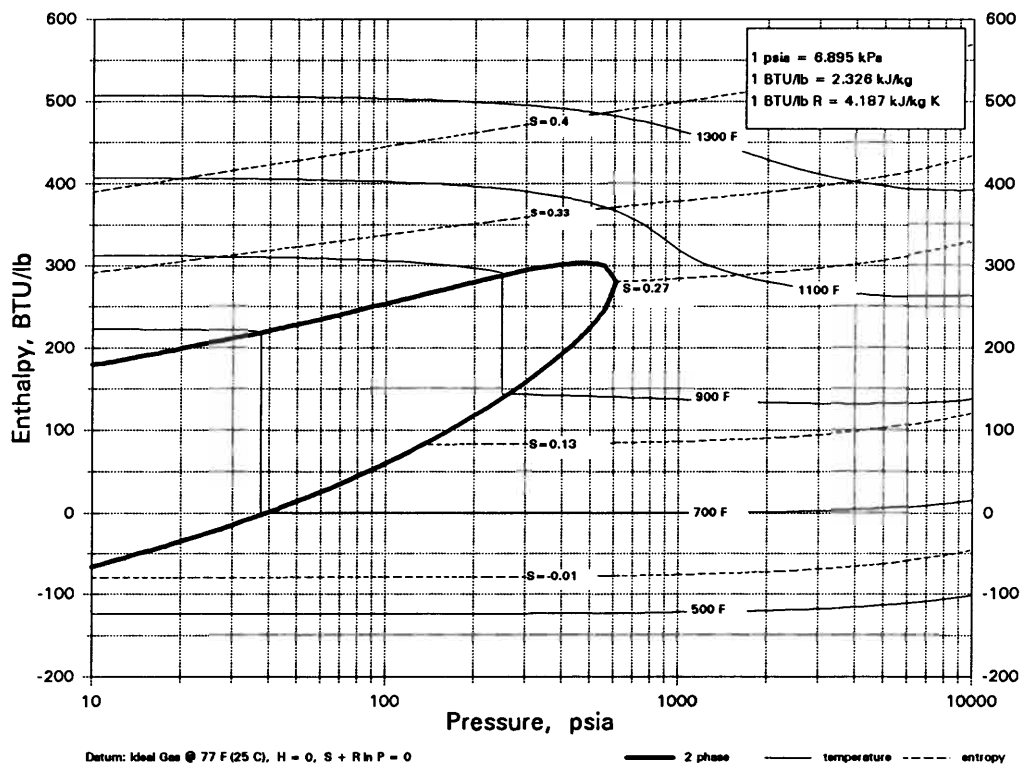
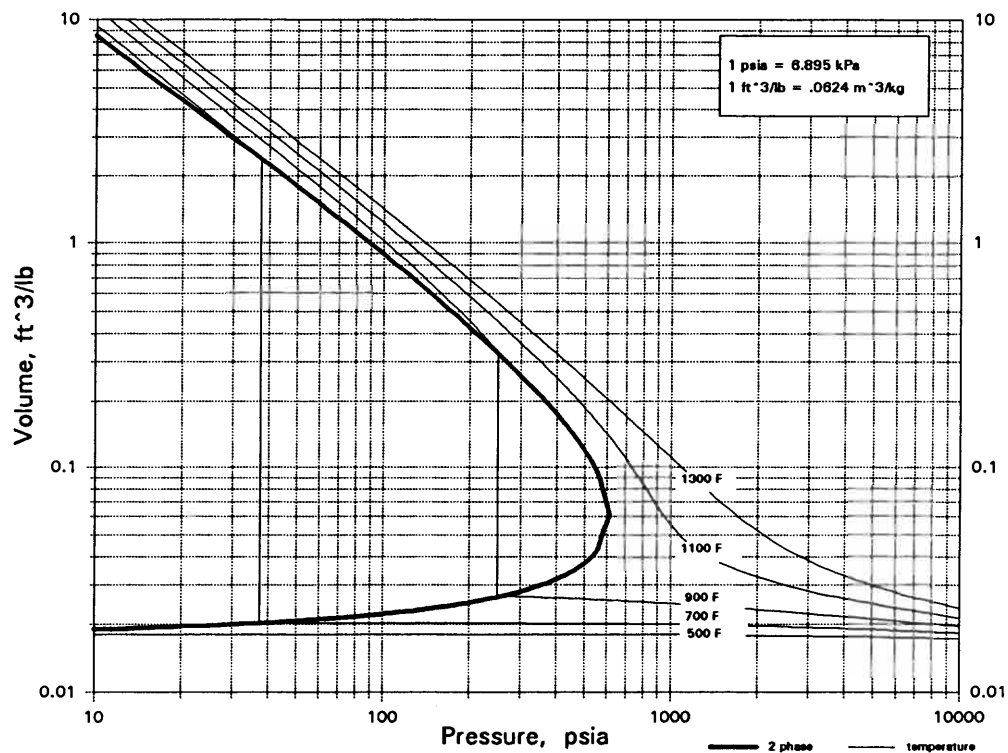
C5H6O4

CITRACONIC ACID



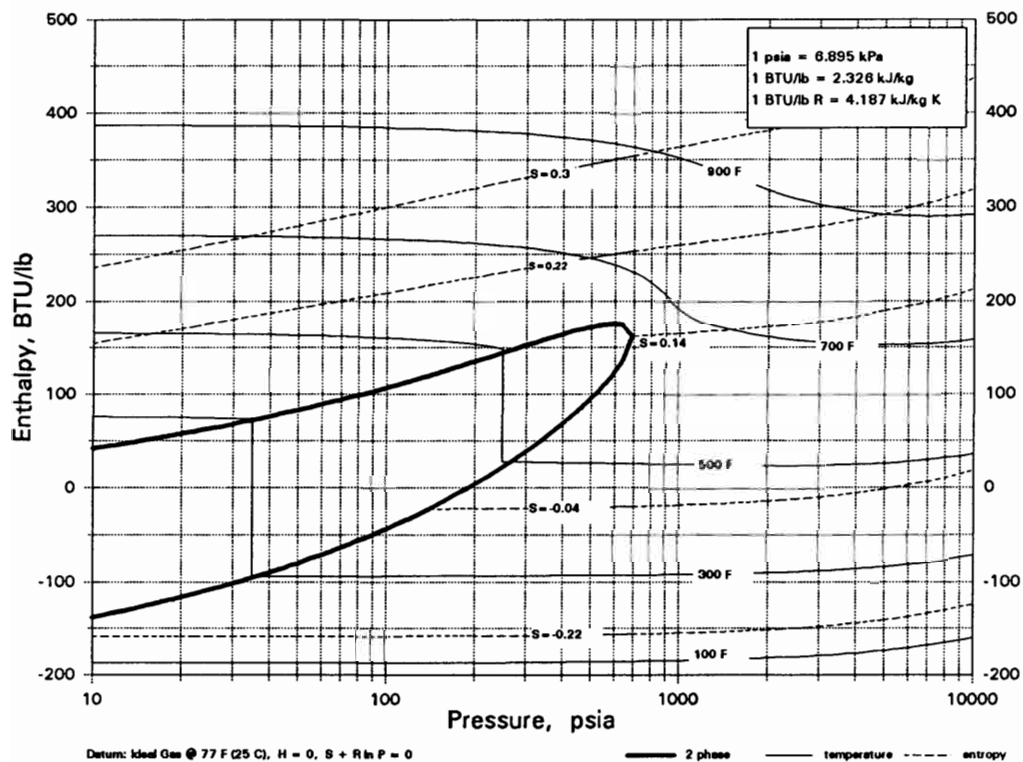
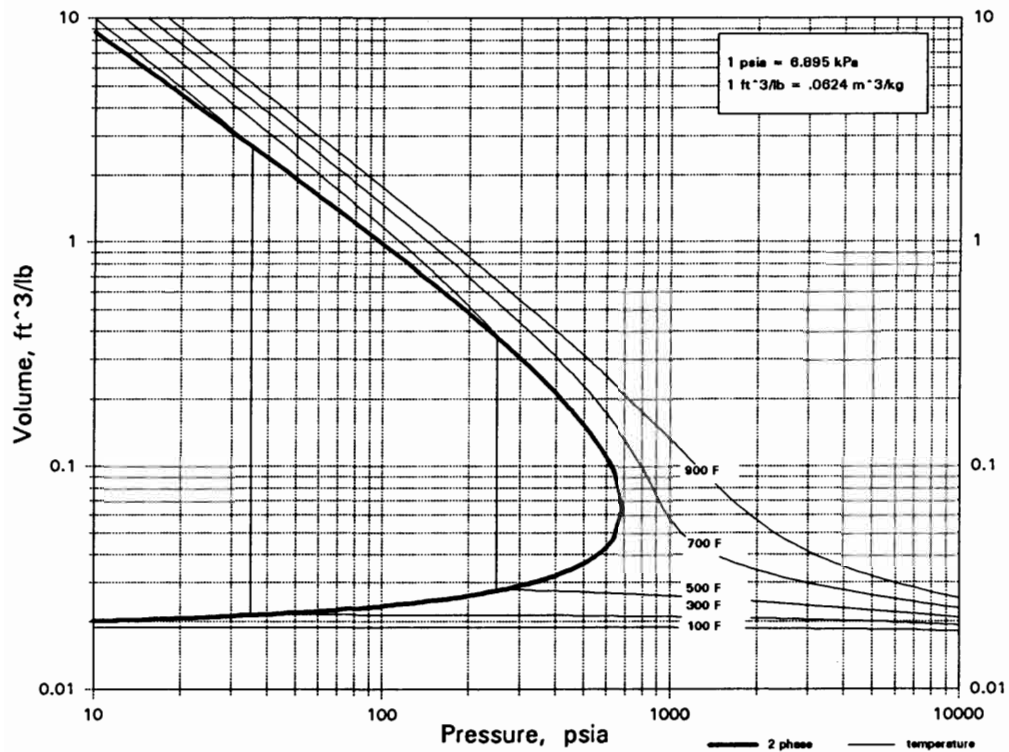
C5H6O4

ITACONIC ACID



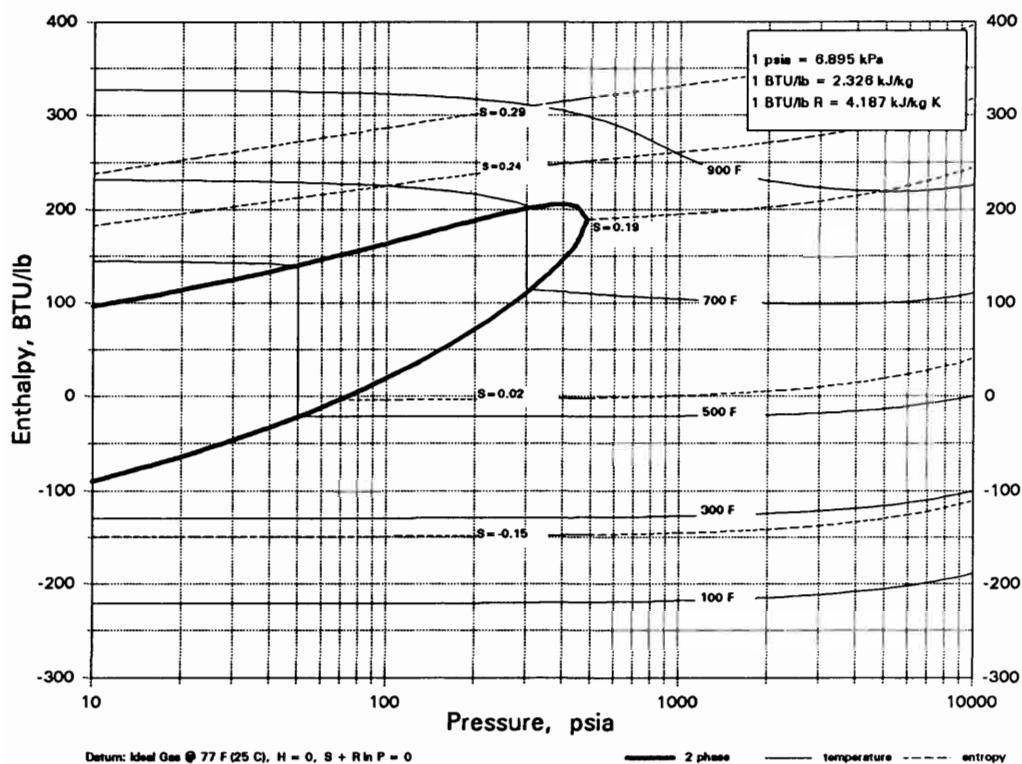
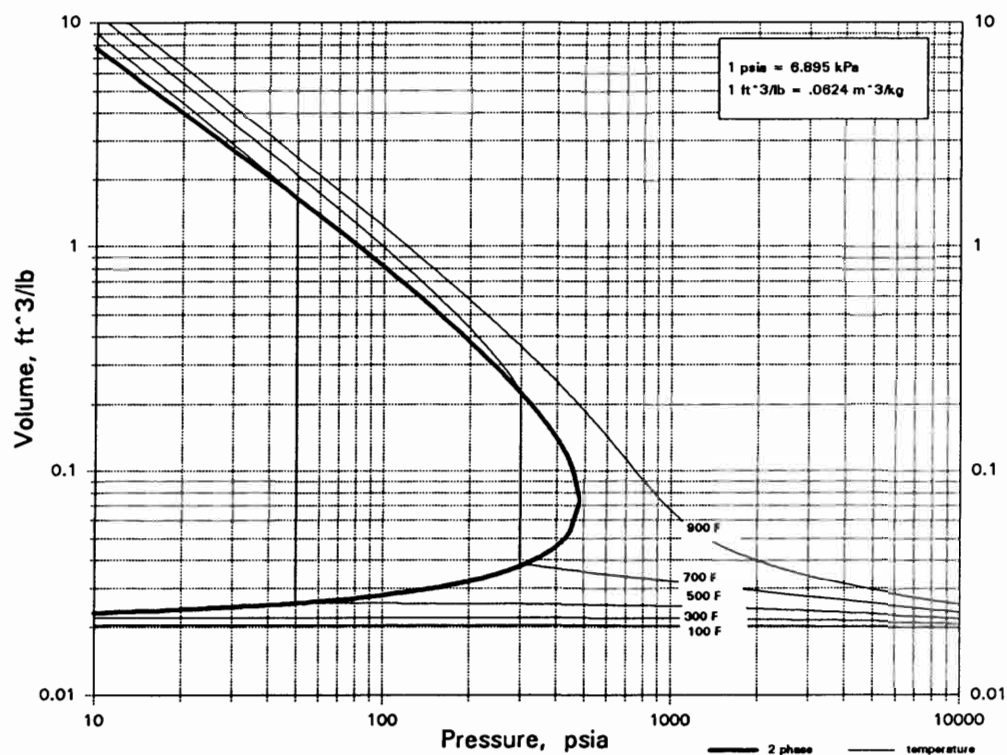
C5H7N

N-METHYLPYRROLE



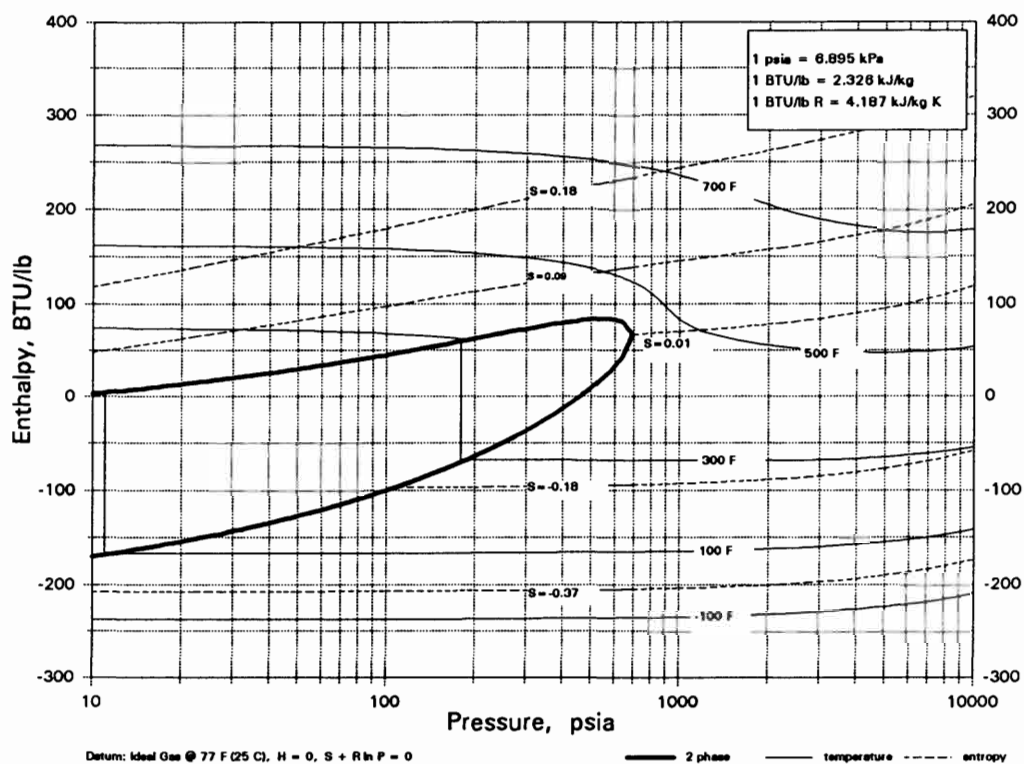
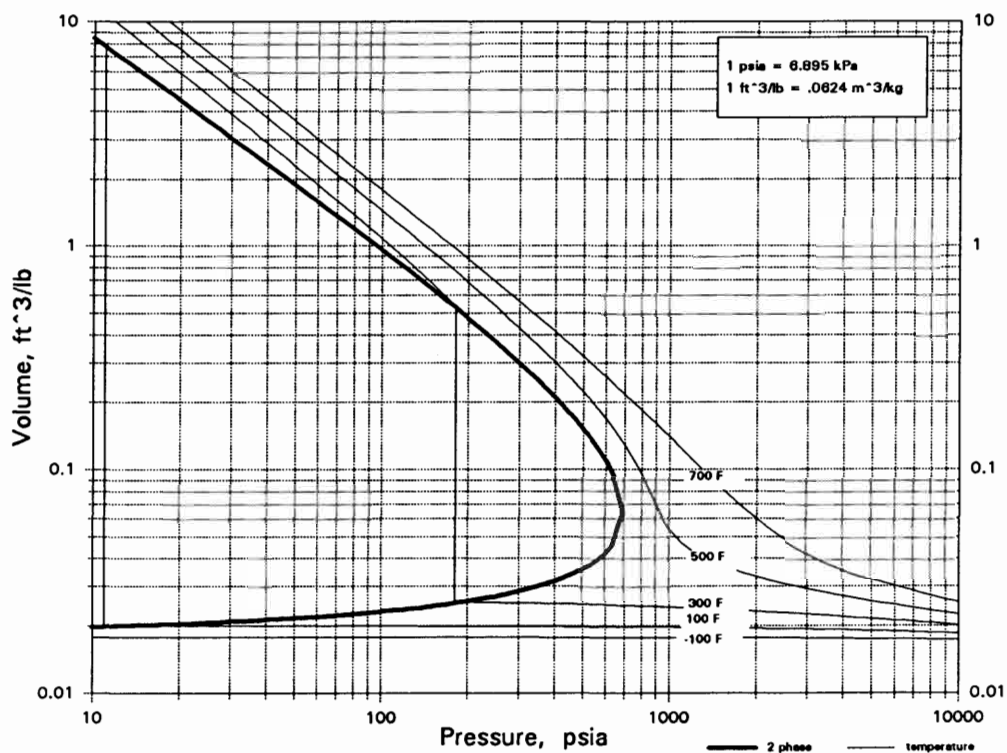
C5H7NO2

ETHYL CYANOACETATE



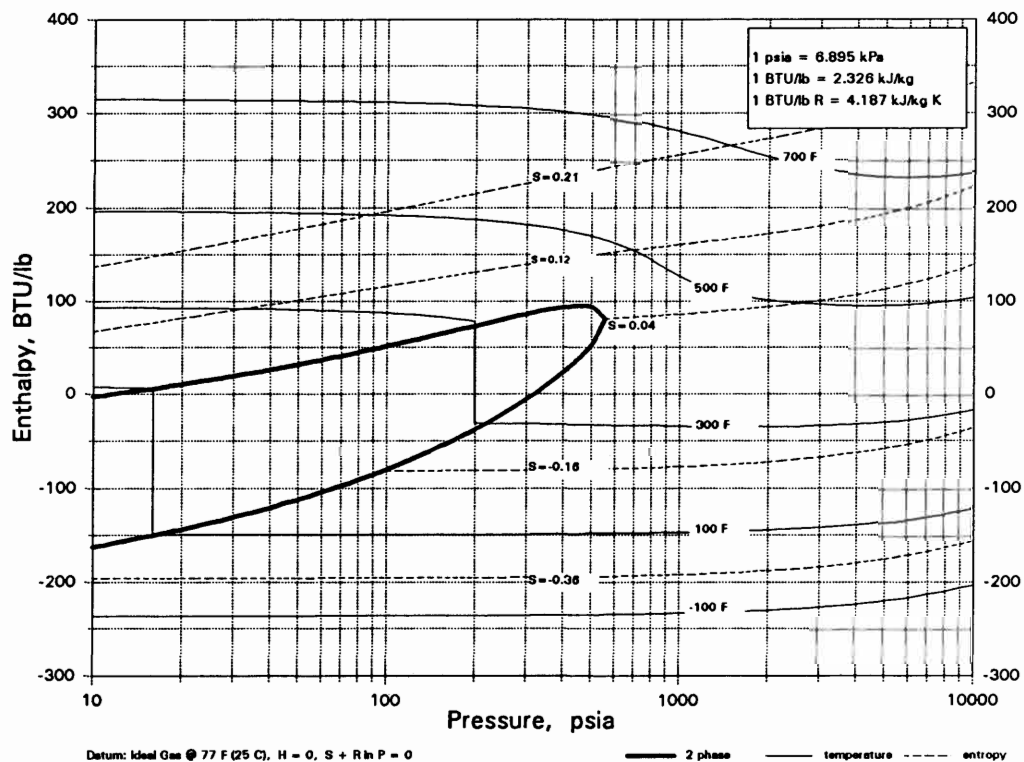
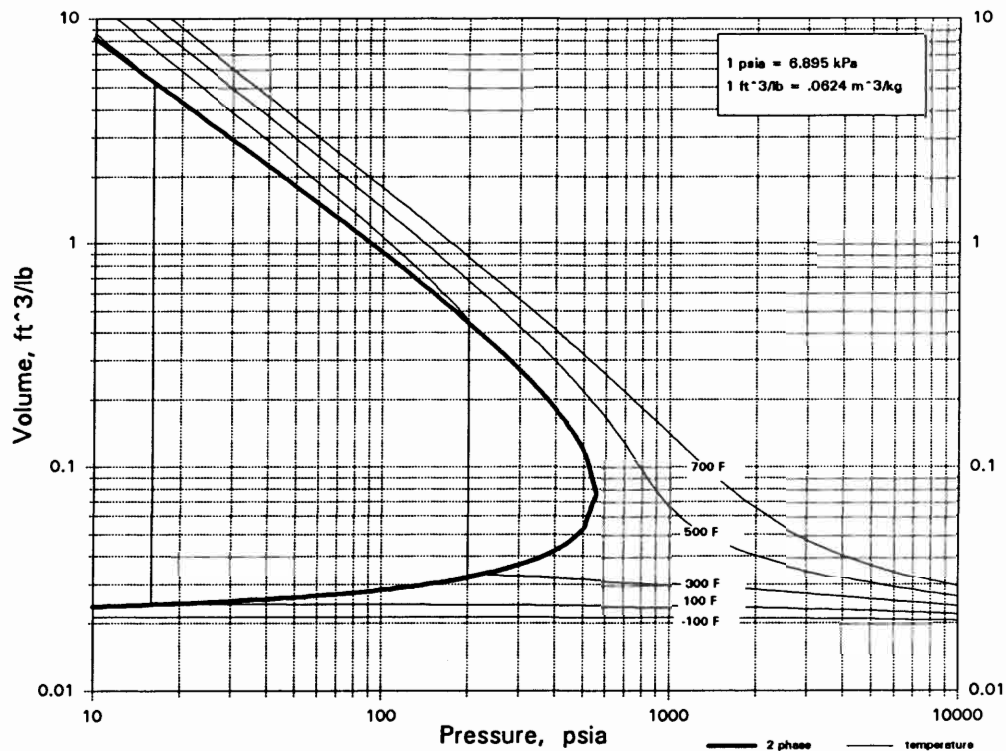
C5H8

CYCLOPENTENE

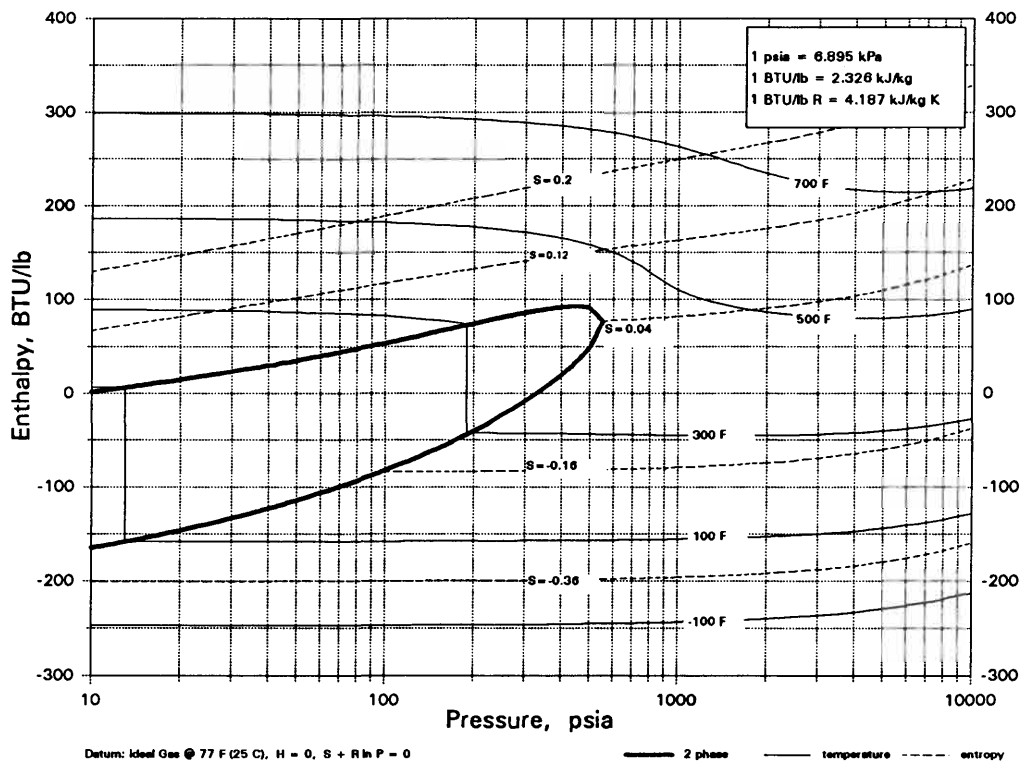
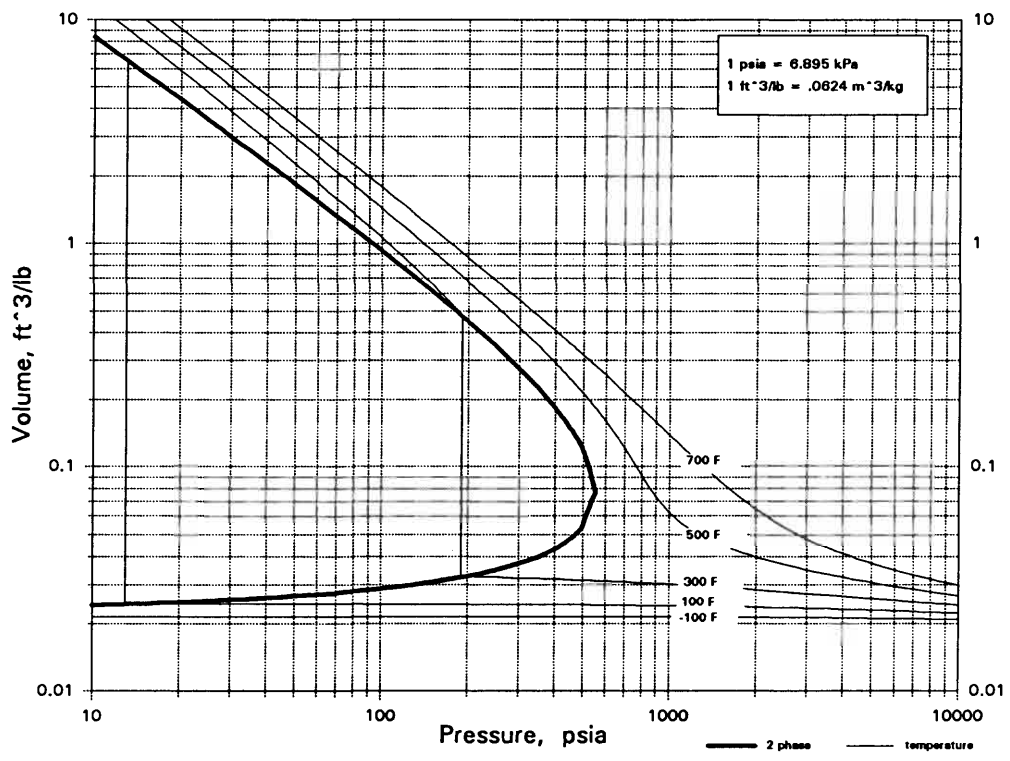


C5H8

ISOPRENE

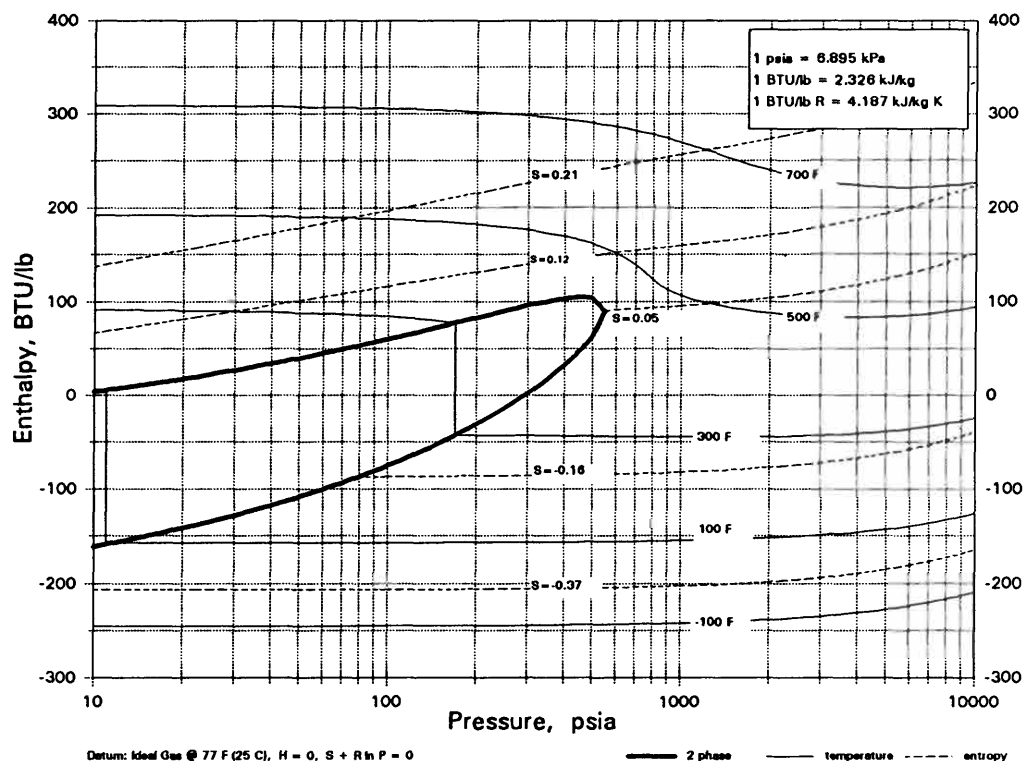
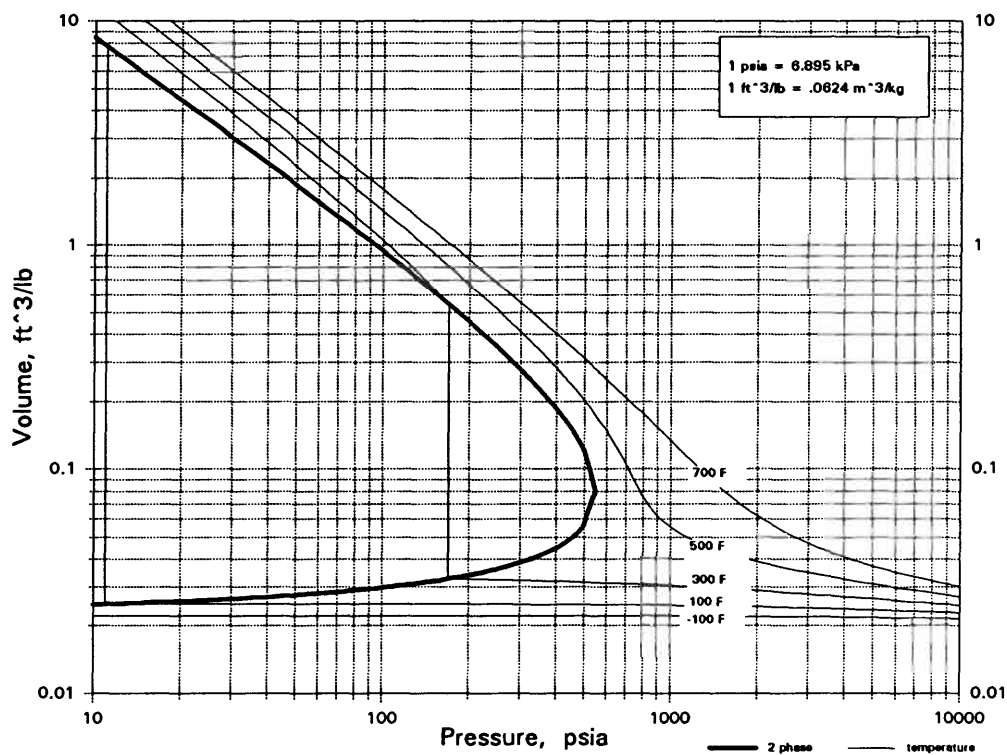


C5H8
3-METHYL-1-2-BUTADIENE

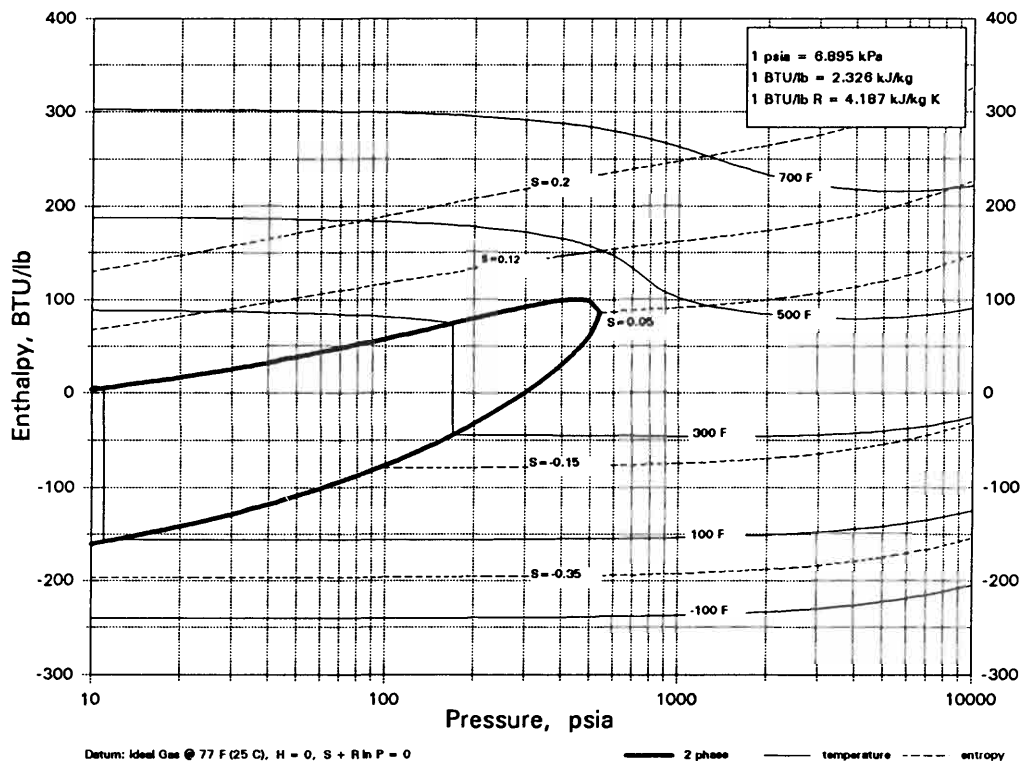
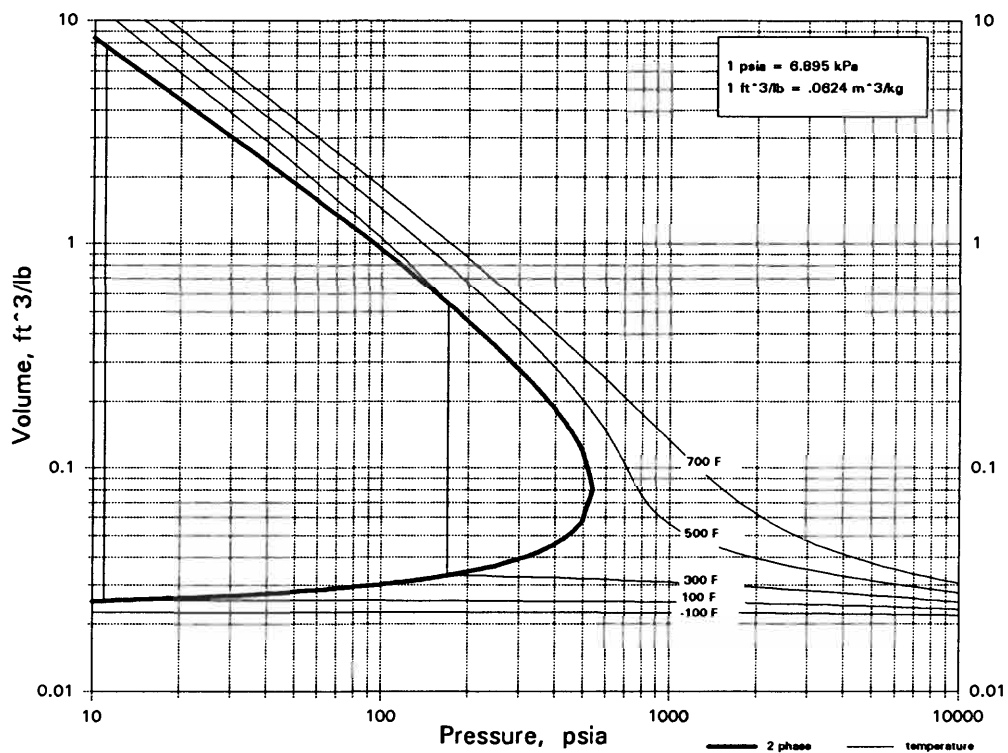


C5H8

1-2-PENTADIENE

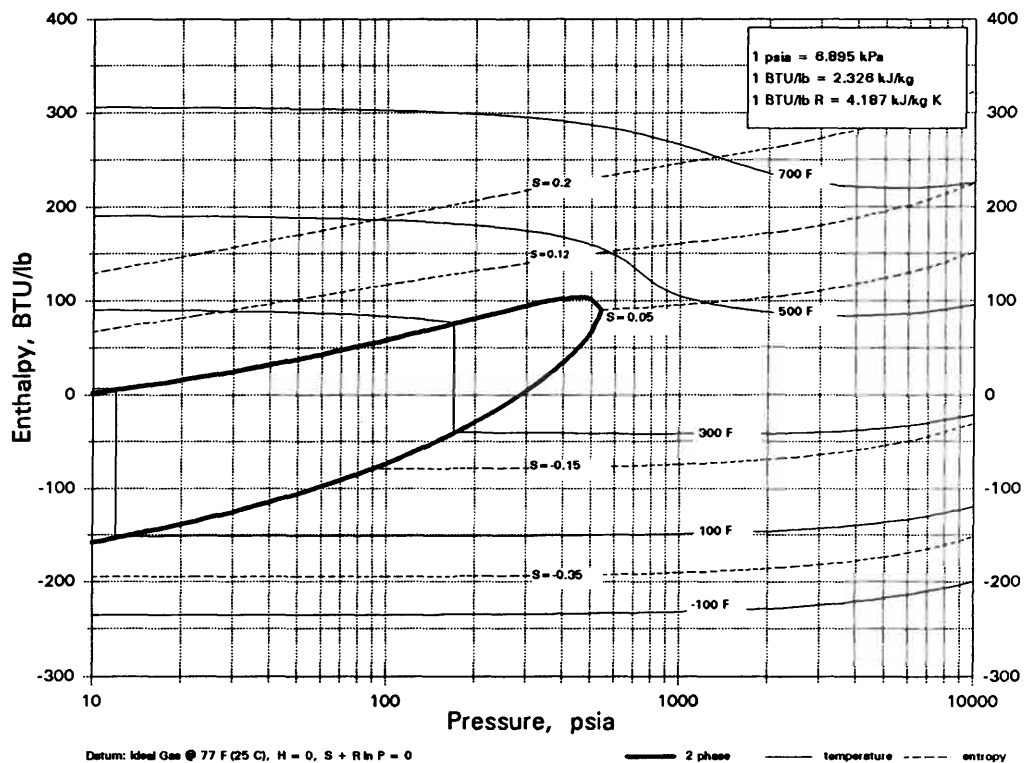
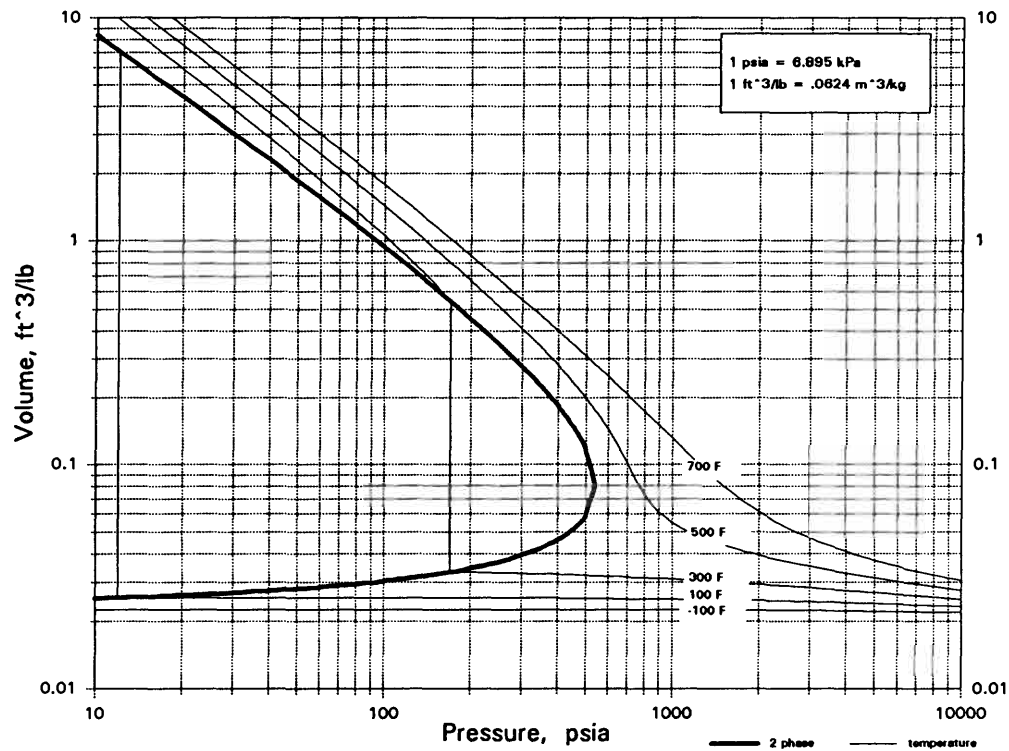


C5H8
cis-1-3-PENTADIENE



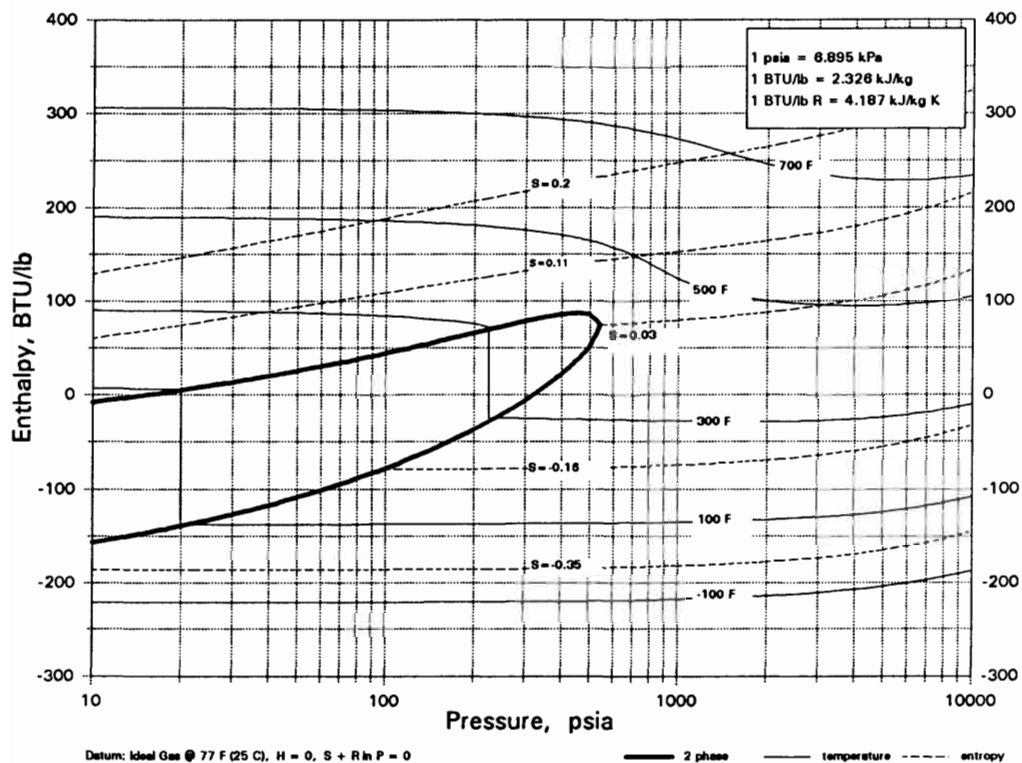
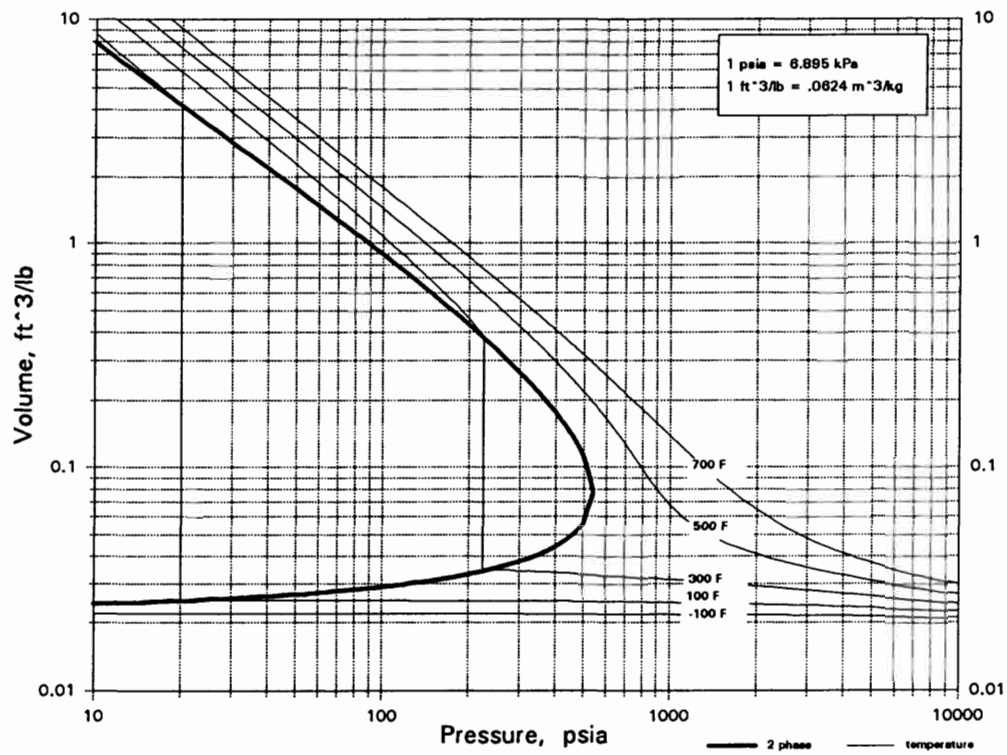
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trans-1-3-PENTADIENE



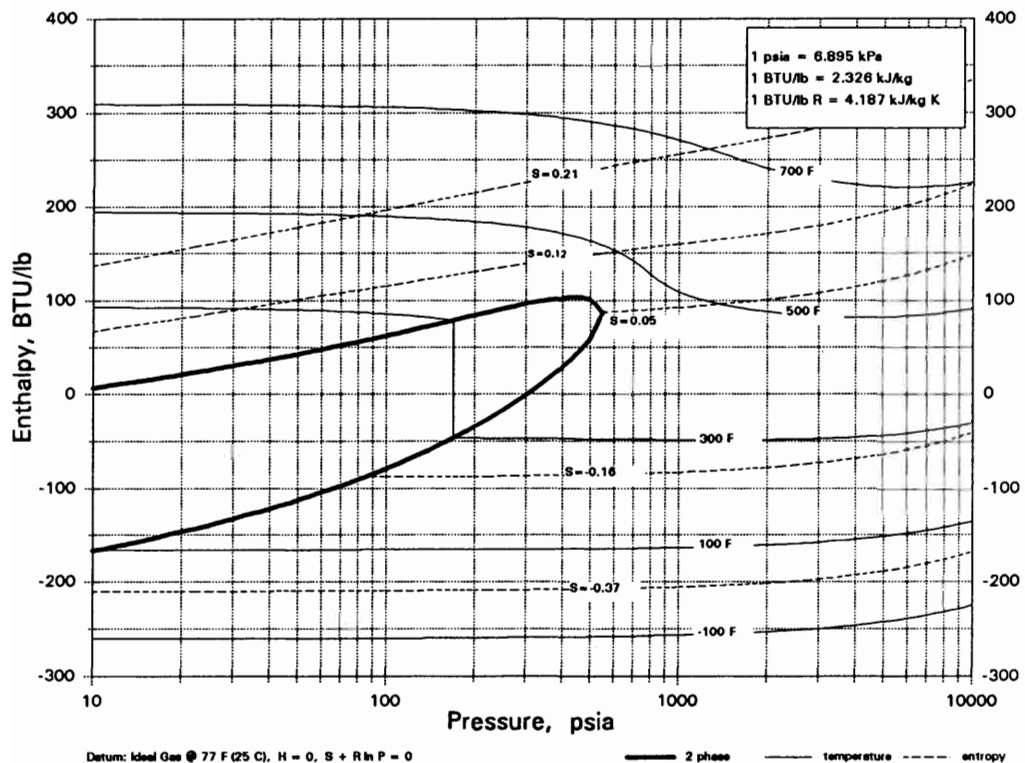
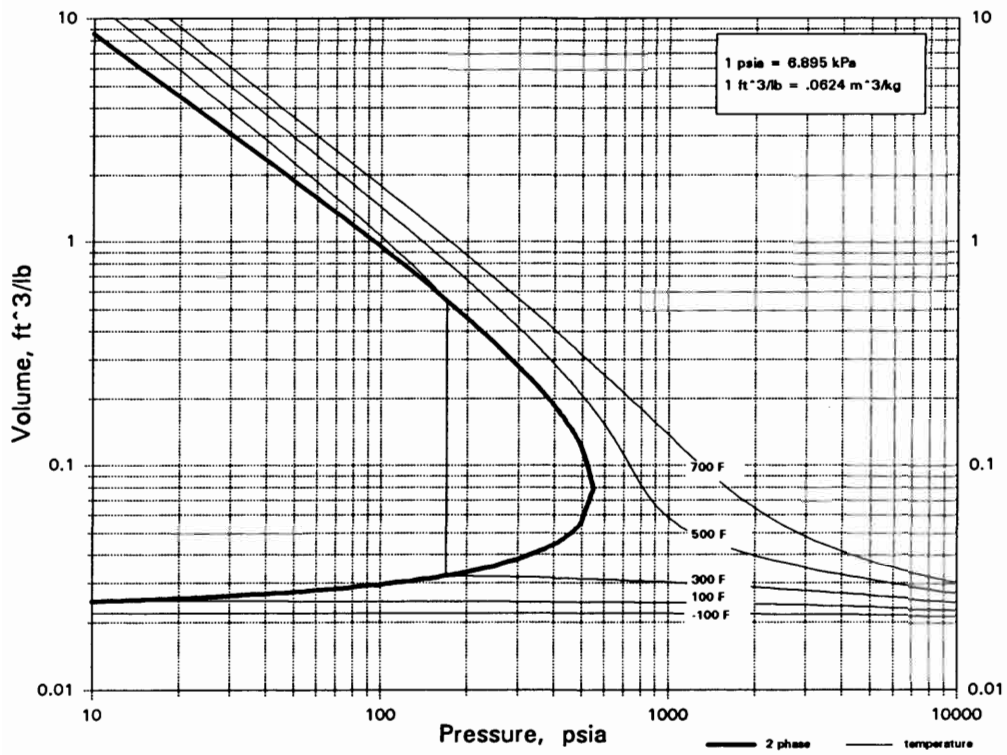
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1-4-PENTADIENE



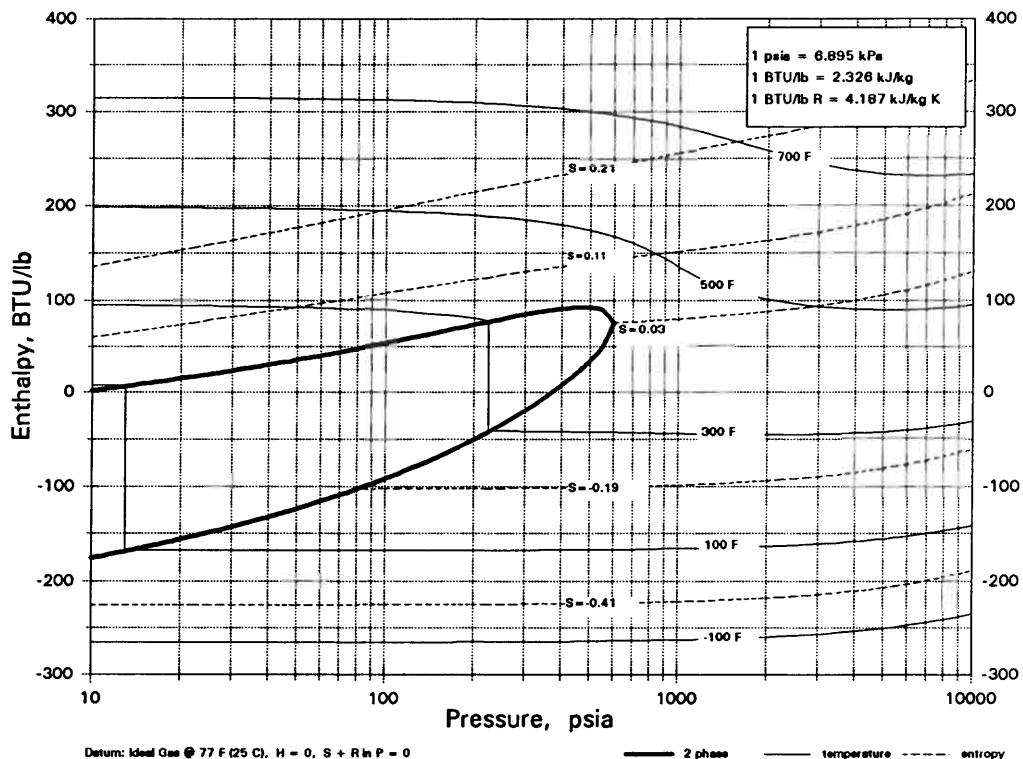
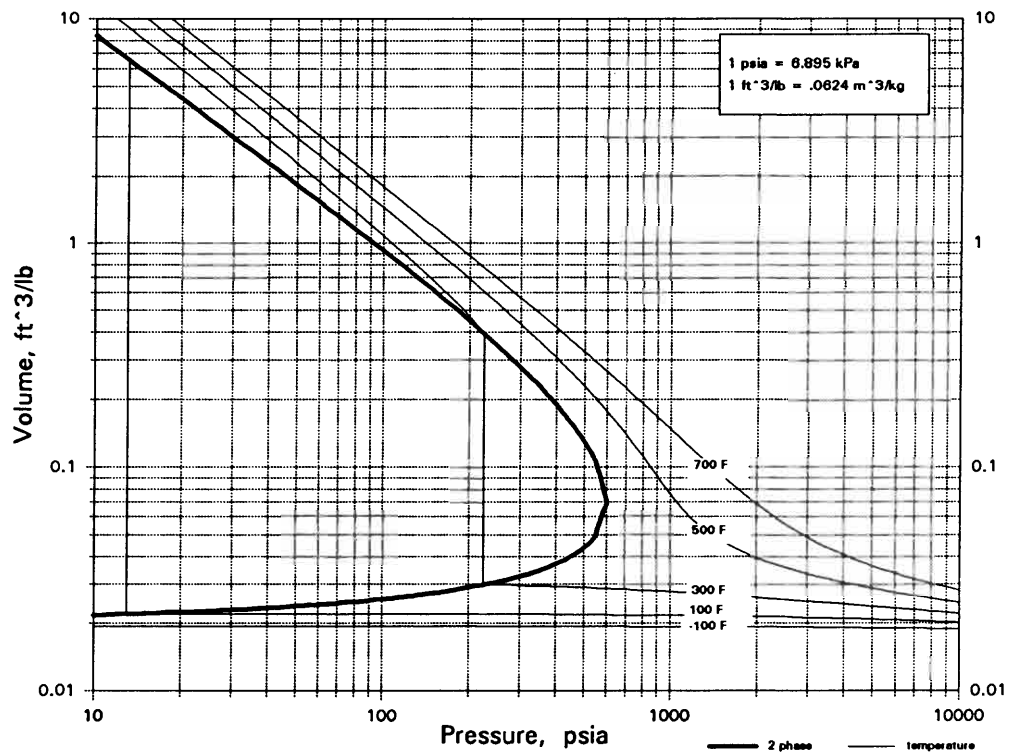
C5H8

2-3-PENTADIENE



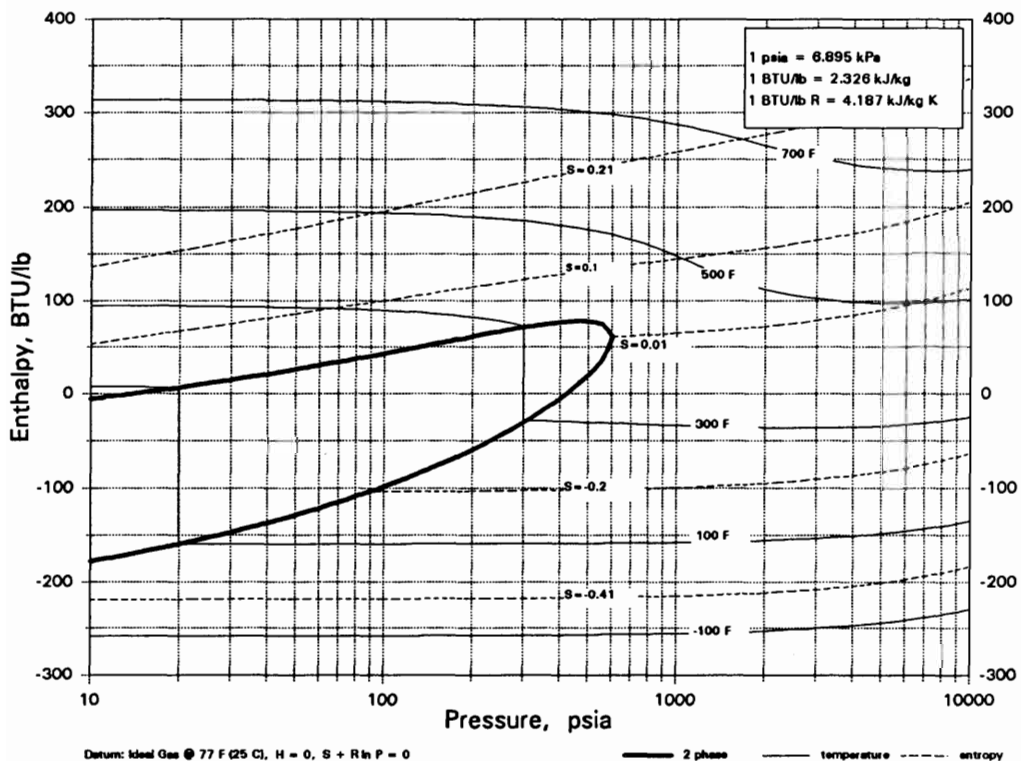
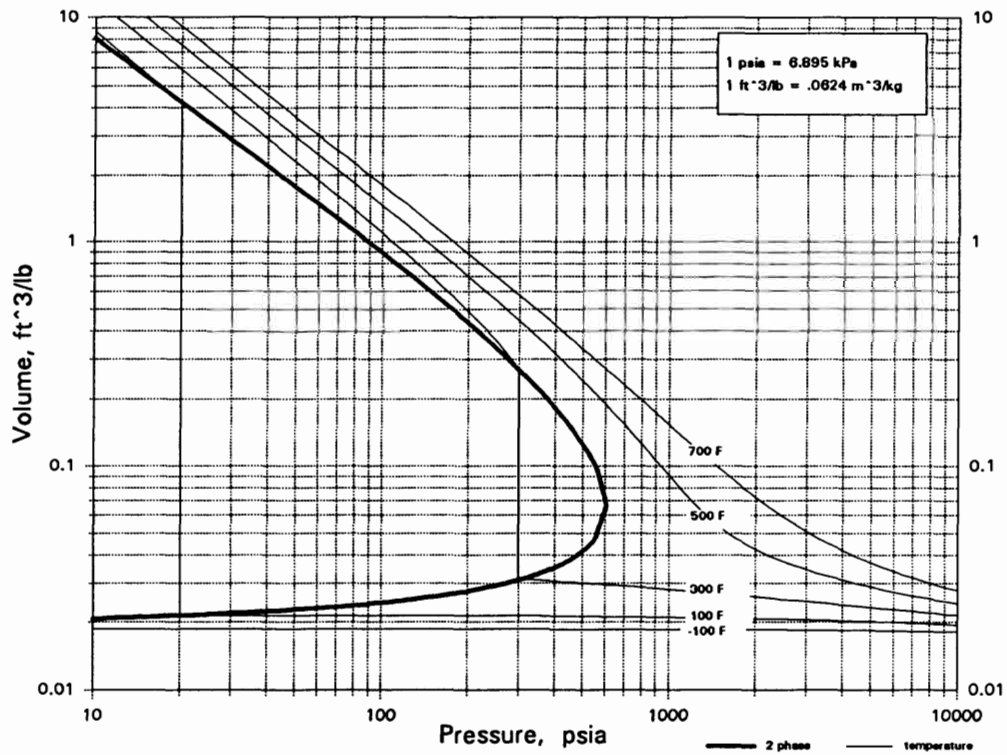
C5H8

1-PENTYNE

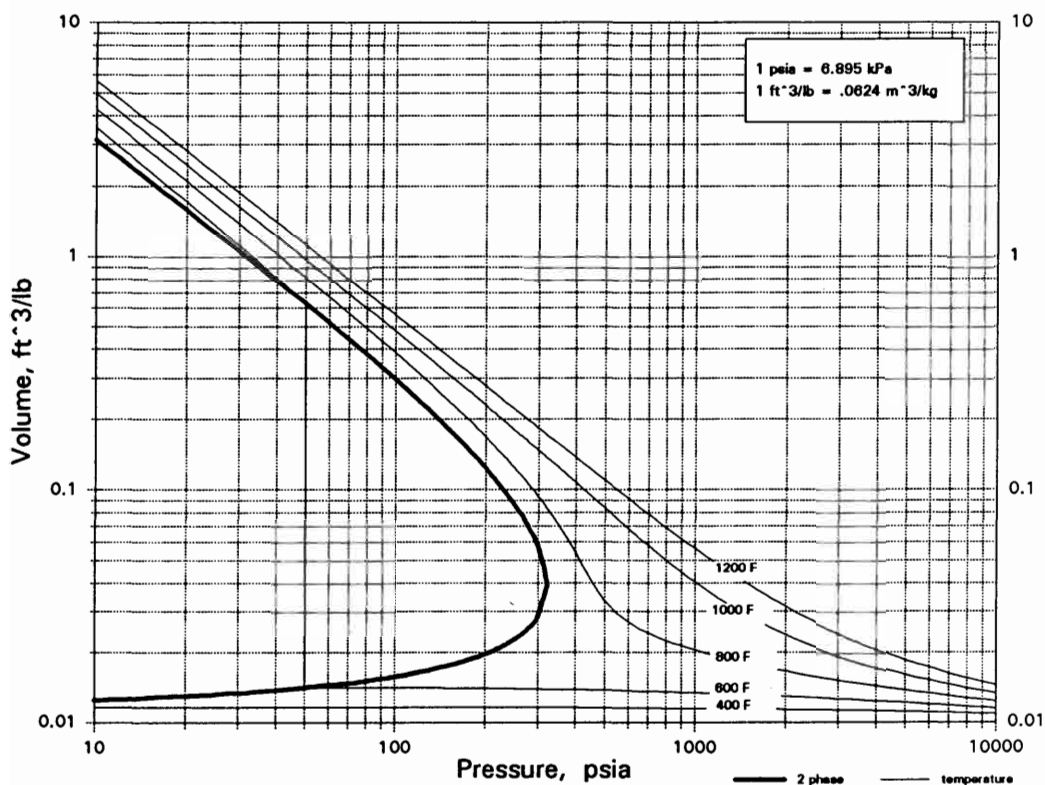


C5H8

3-METHYL-1-BUTYNE



C5H8N4O12 PENTAERYTHRITOL TETRANITRATE

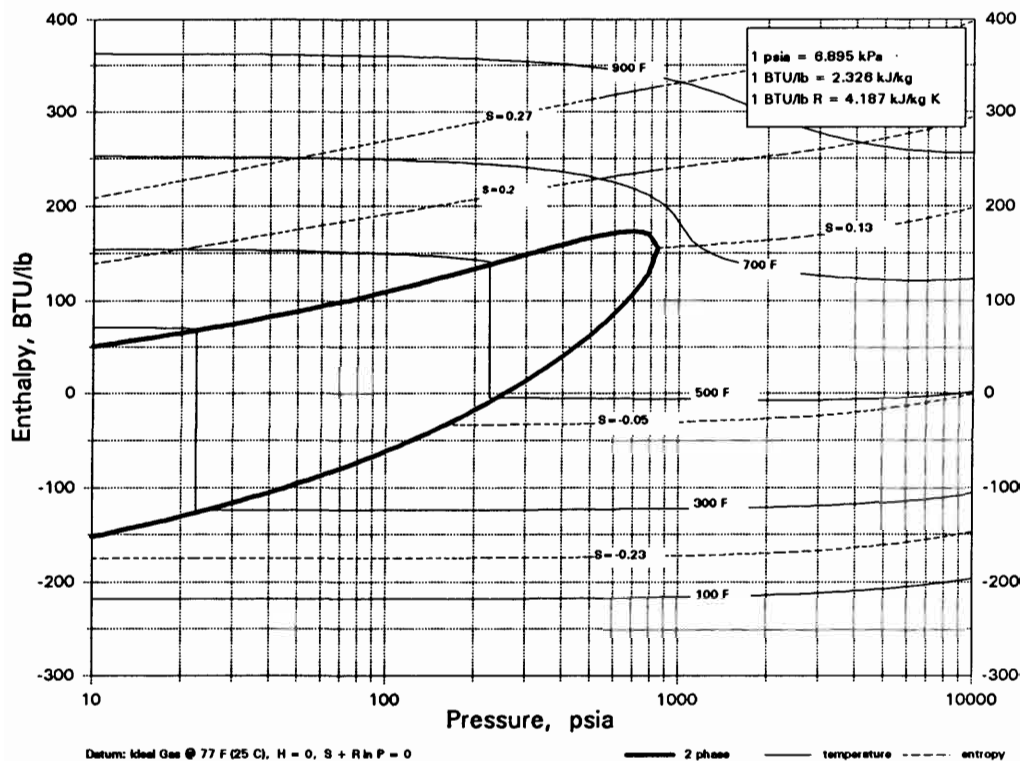
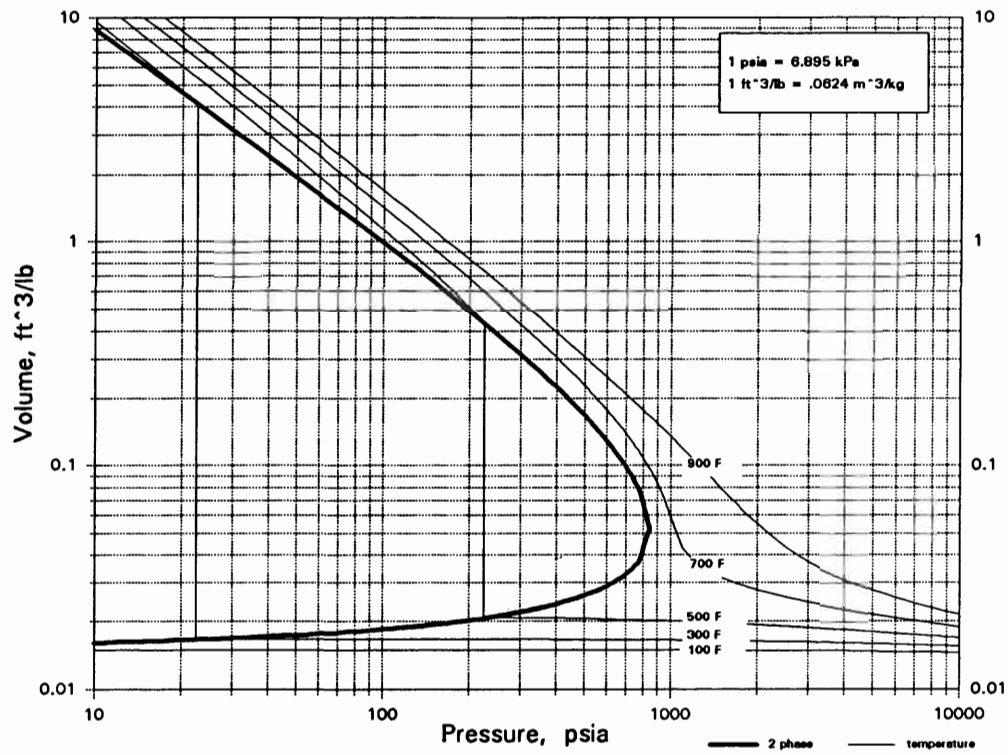


1. Boiling Point, K..... 543.00
2. Critical Temperature, K.... 676.00
3. Critical Pressure, atm..... 22.11

Heat capacity data are not available.

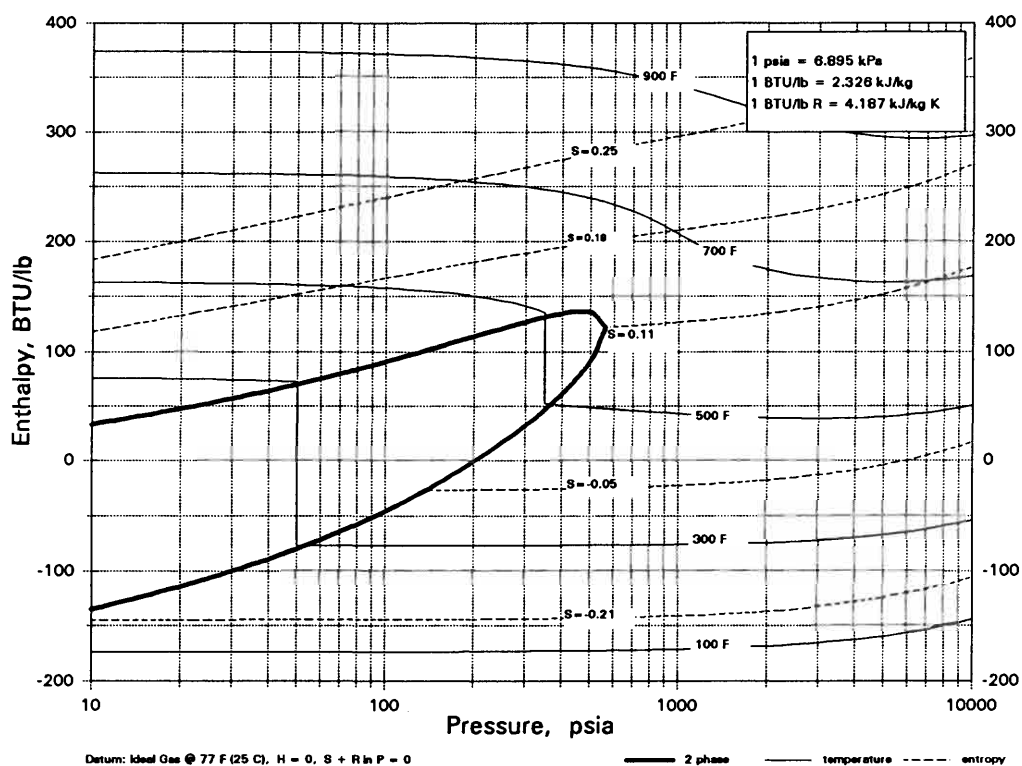
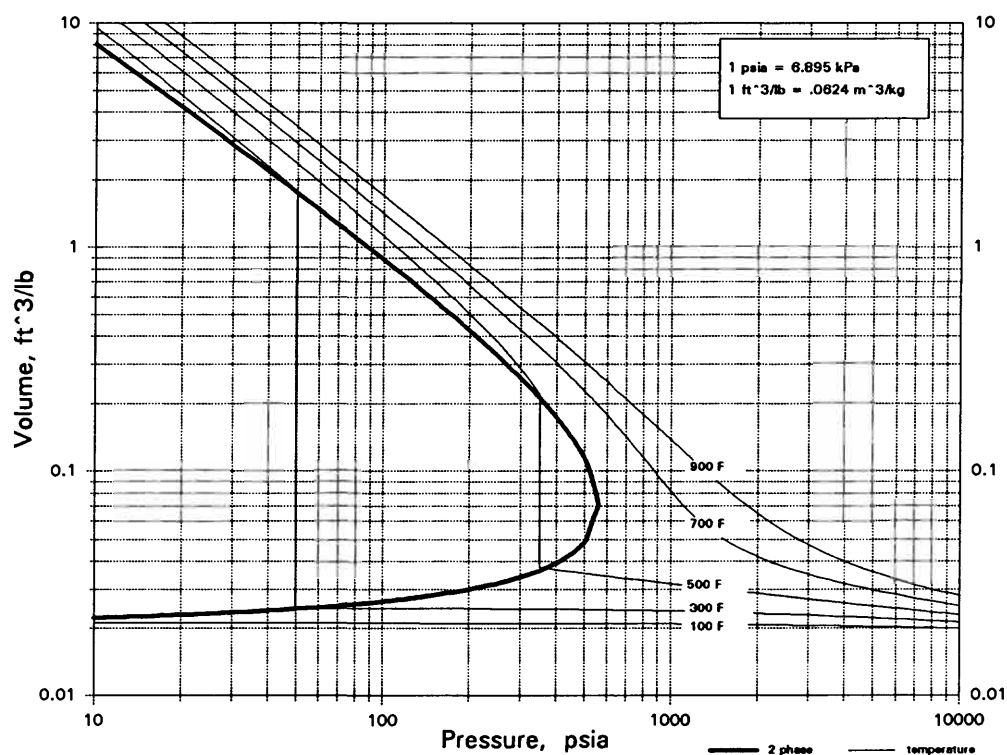
C5H8O

CYCLOPENTANONE



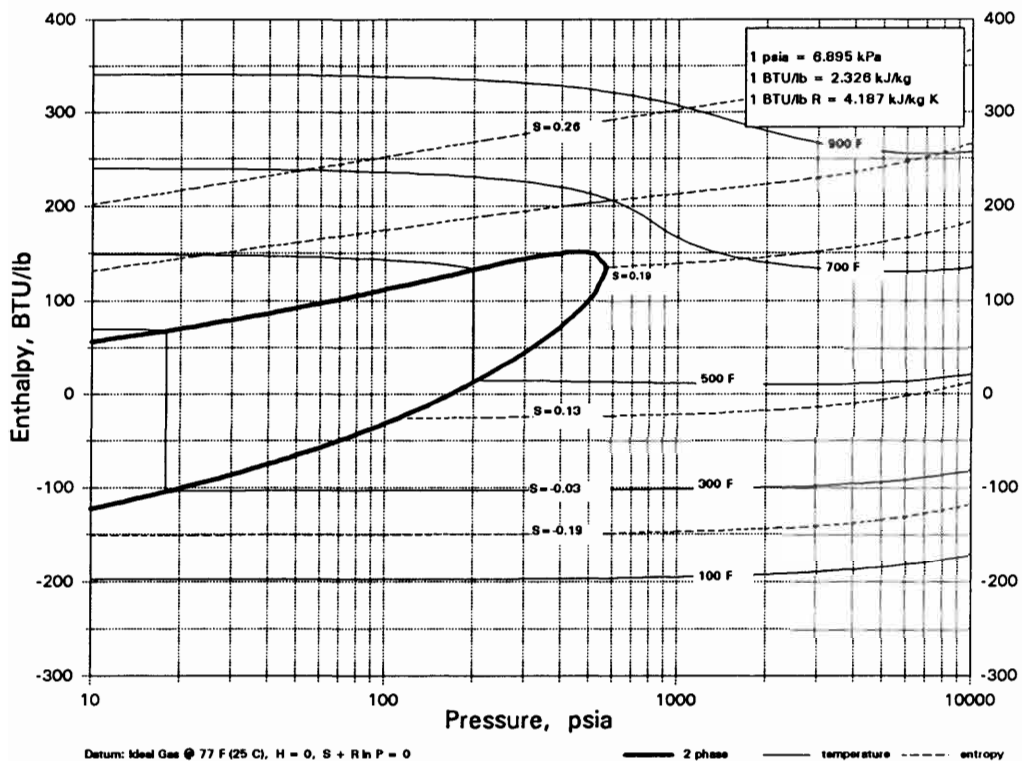
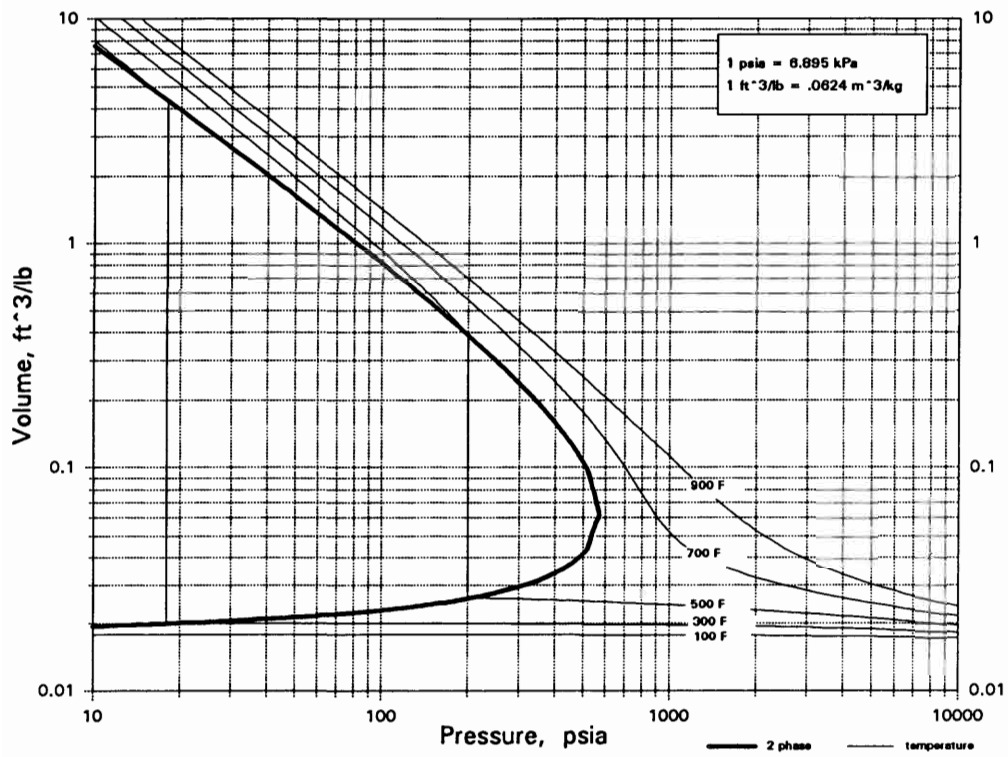
C5H8O

METHYL ISOPROPENYL KETONE



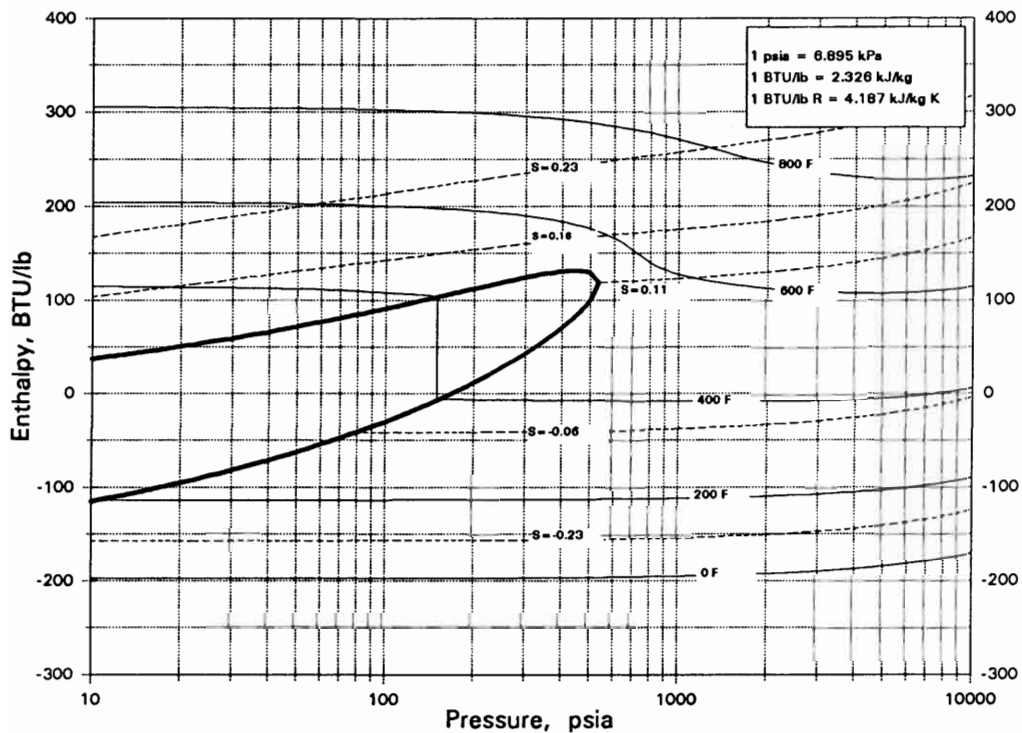
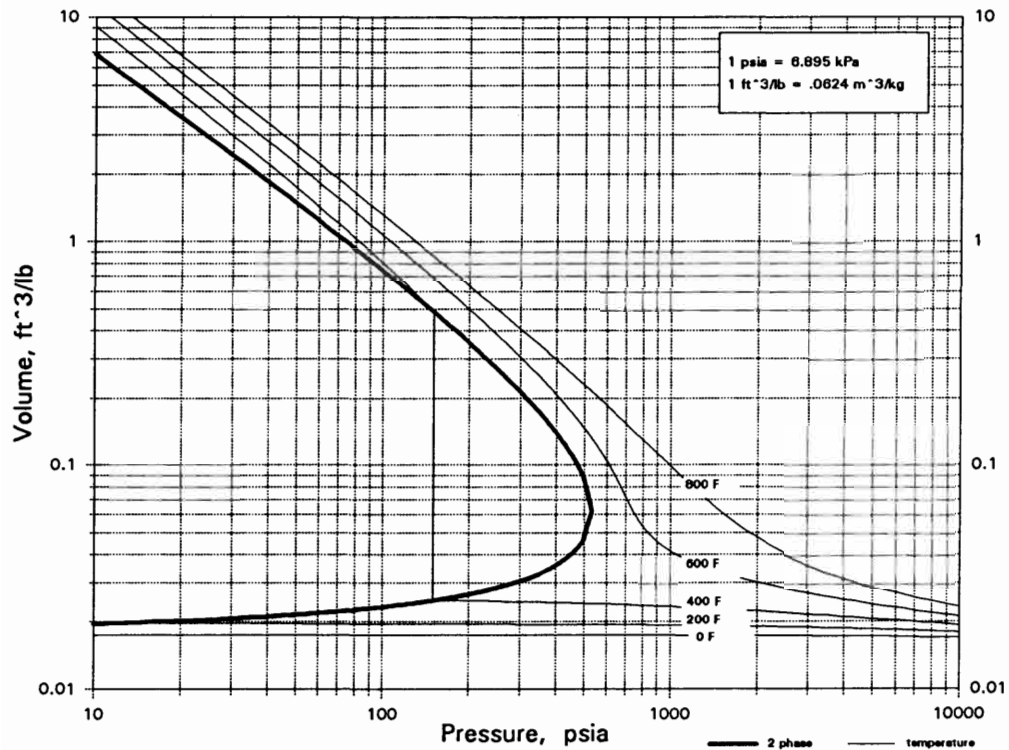
C5H8O2

ACETYLACETONE



C5H8O2

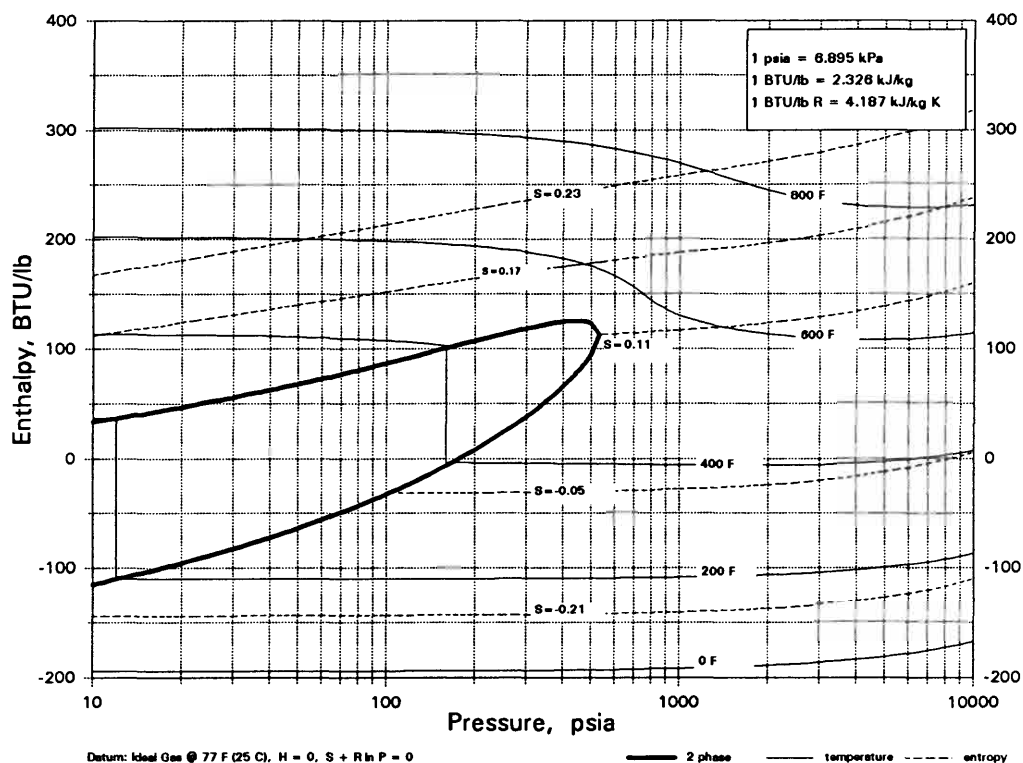
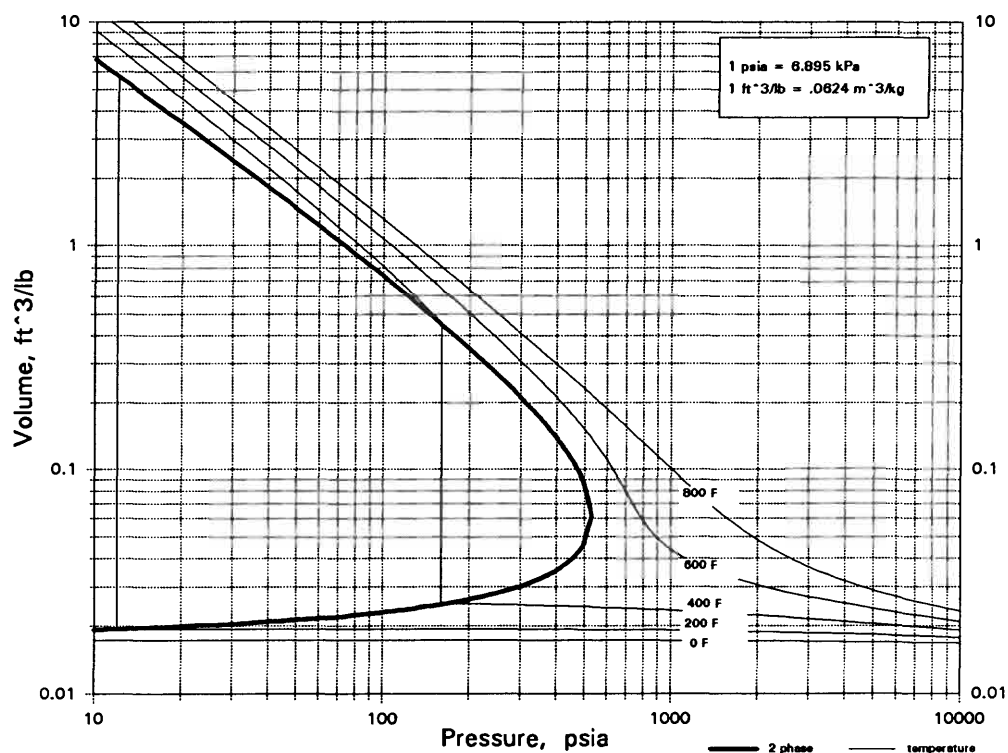
ALLYL ACETATE



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

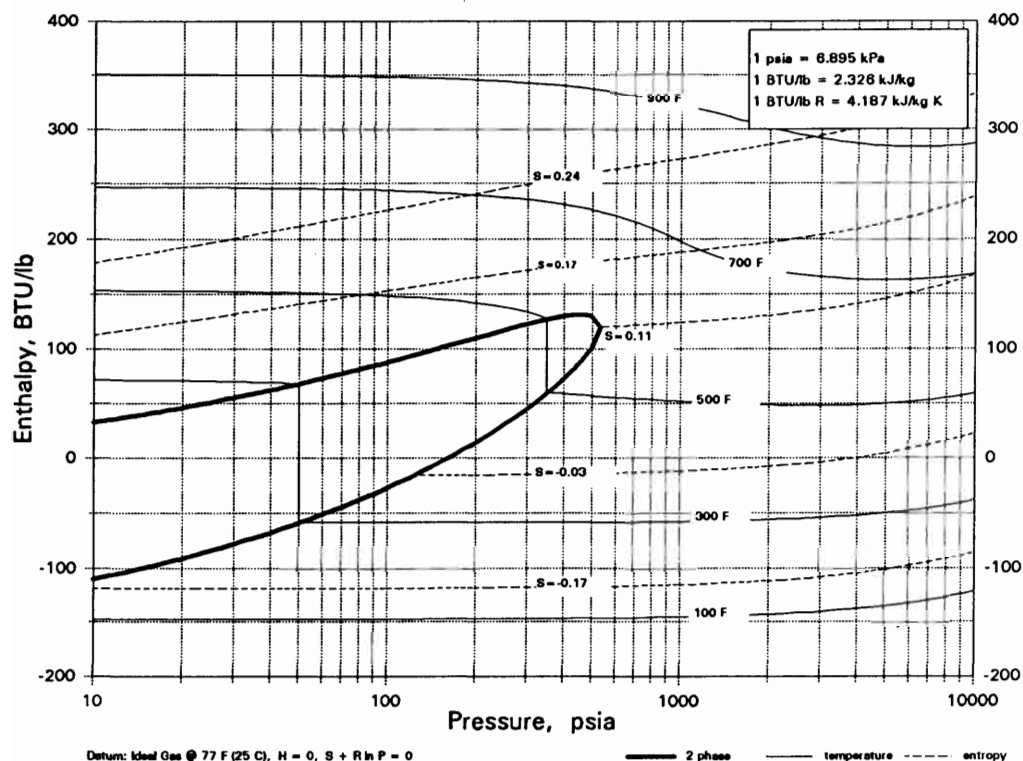
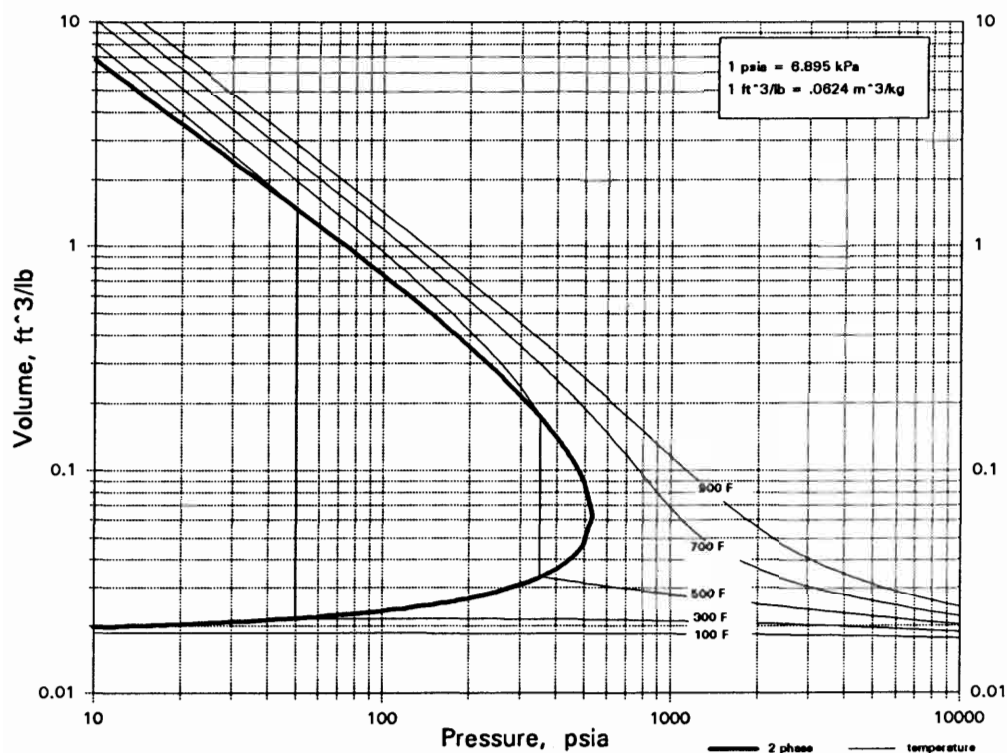
C5H8O2

ETHYL ACRYLATE



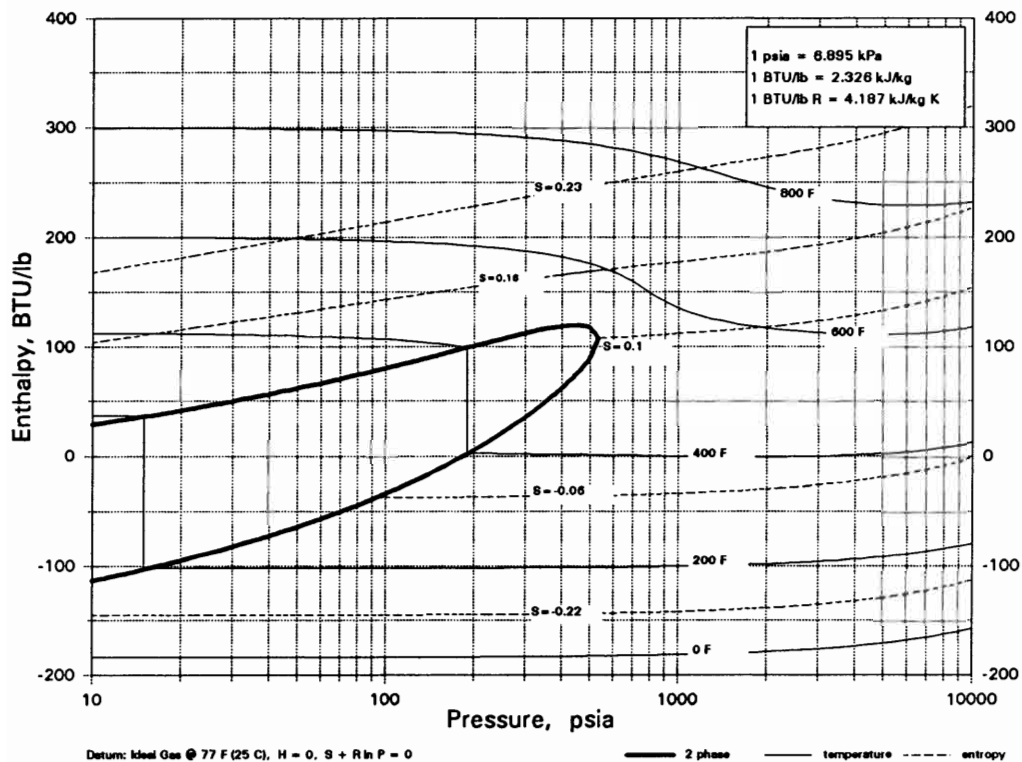
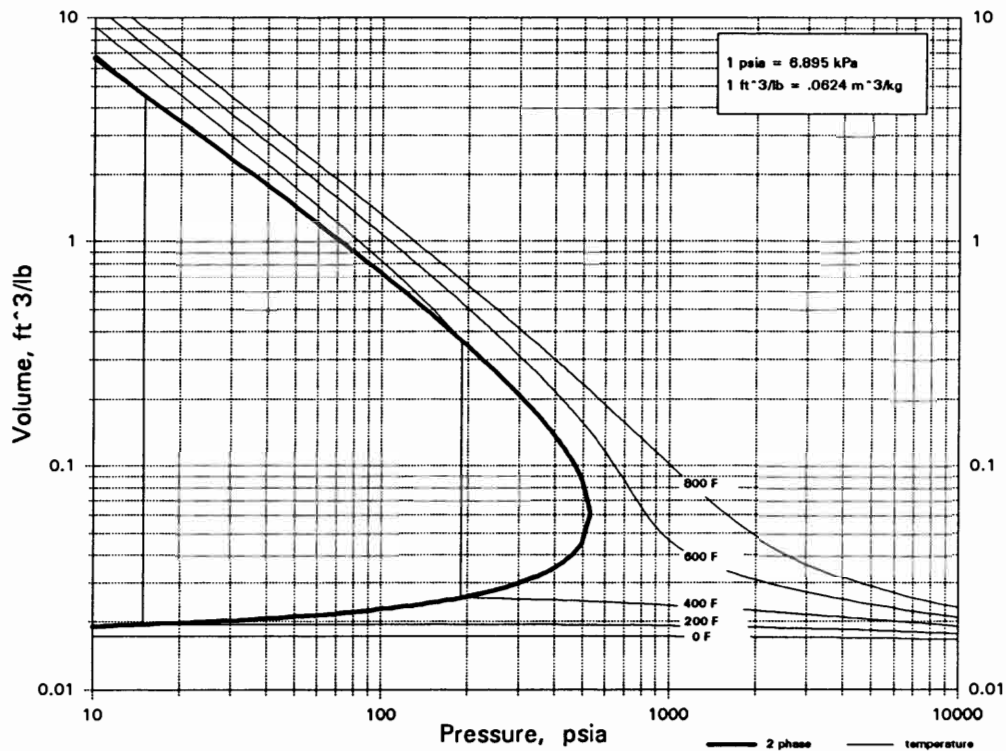
C5H8O2

METHYL METHACRYLATE



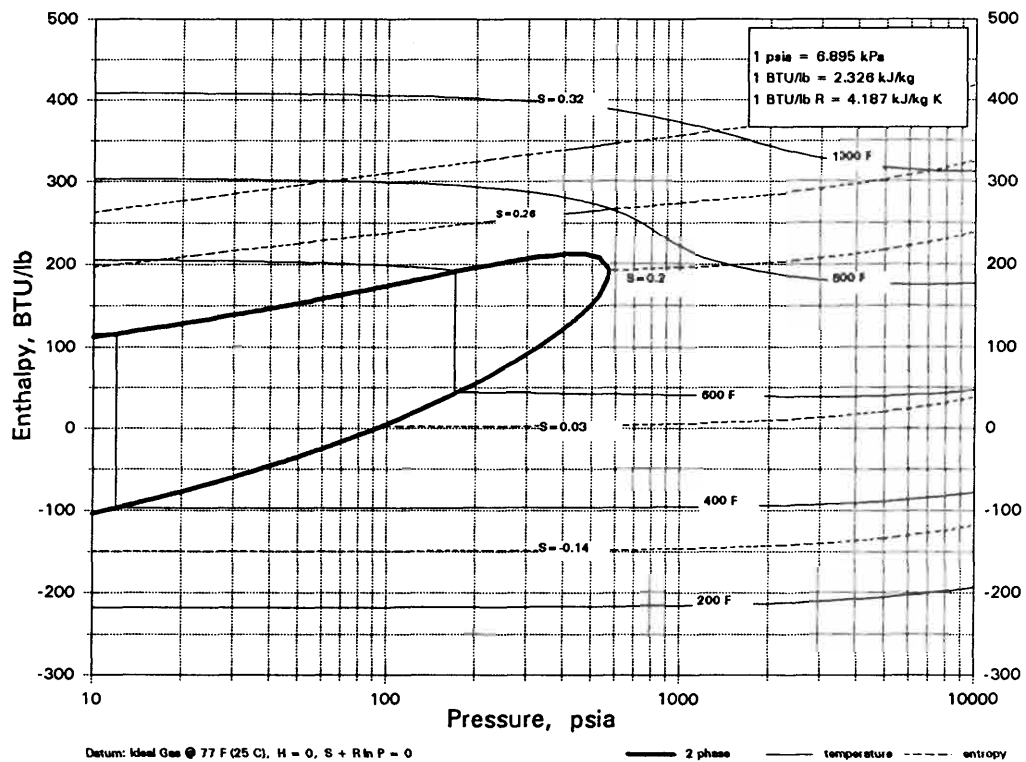
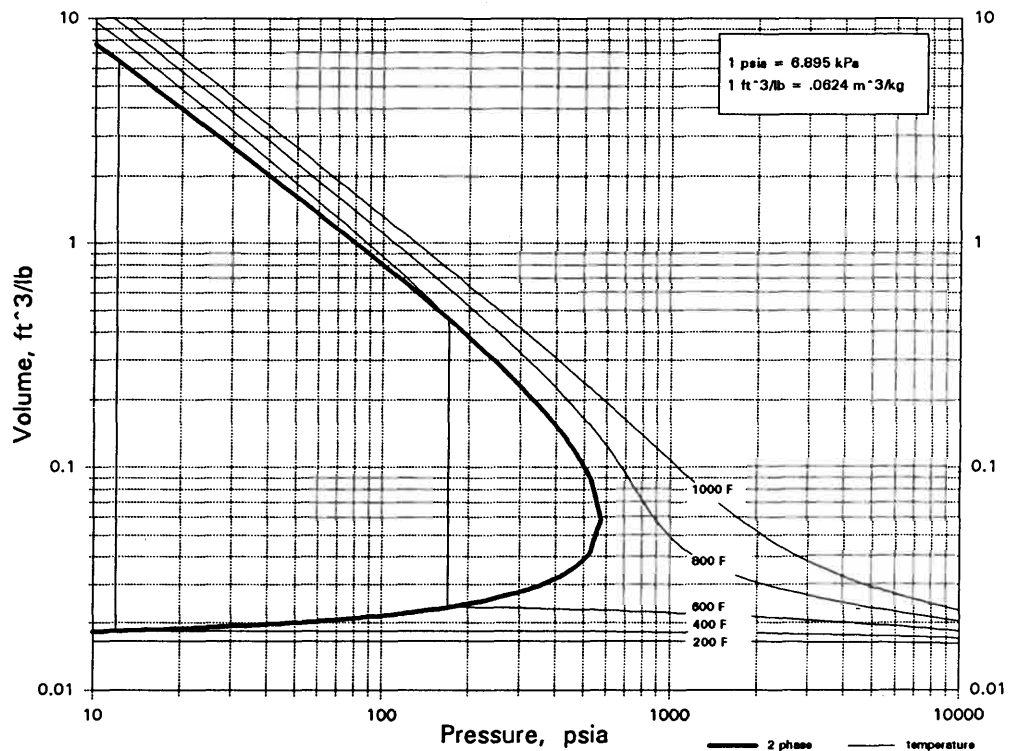
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VINYL PROPIONATE



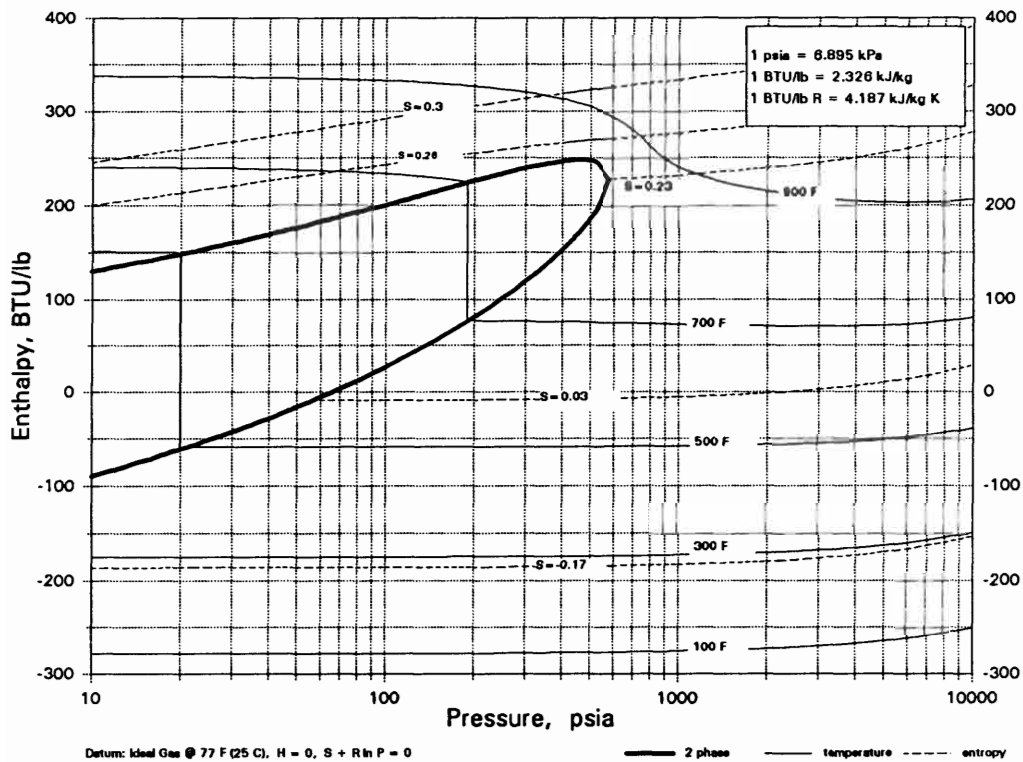
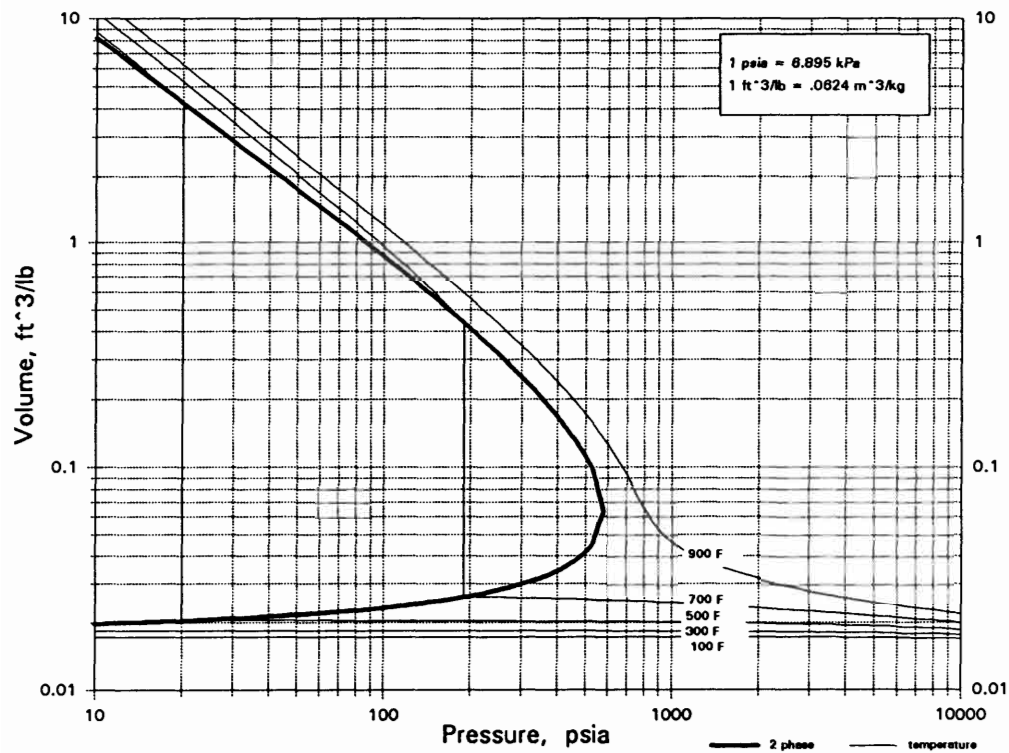
C5H8O3

2-HYDROXYETHYL ACRYLATE



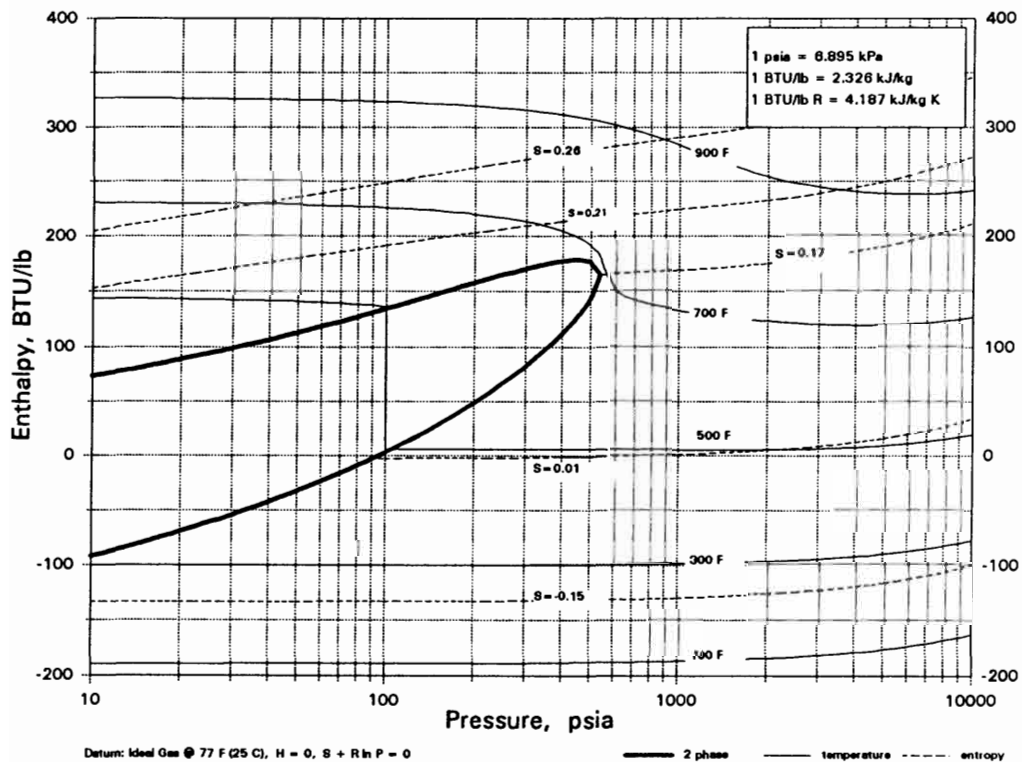
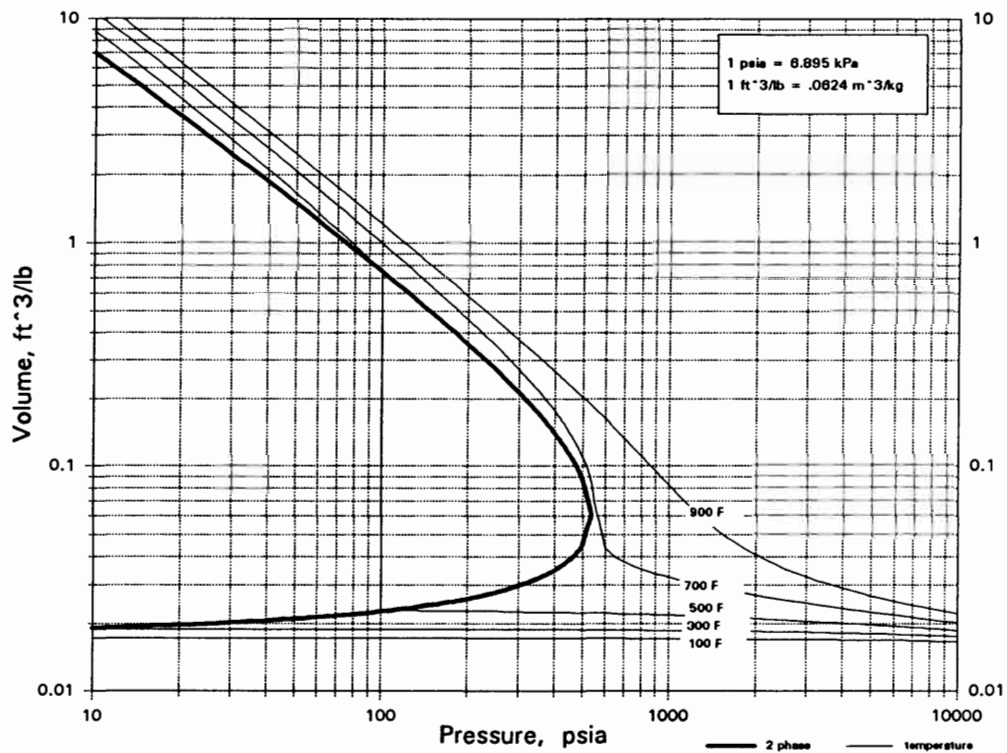
C5H8O3

LEVULINIC ACID



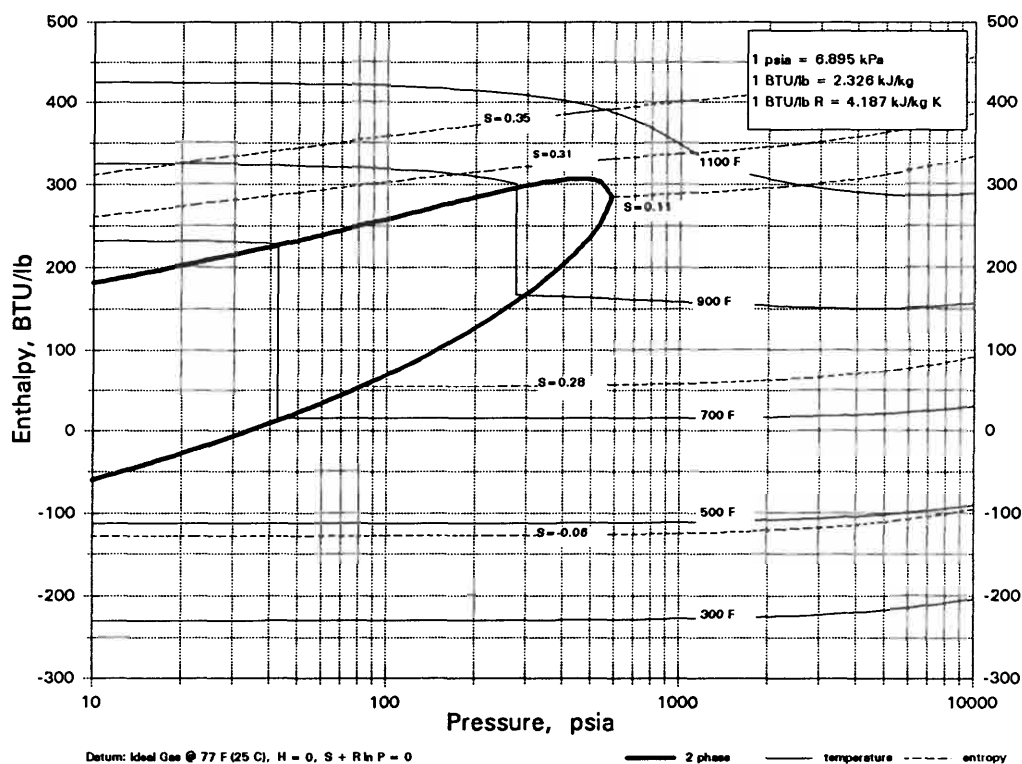
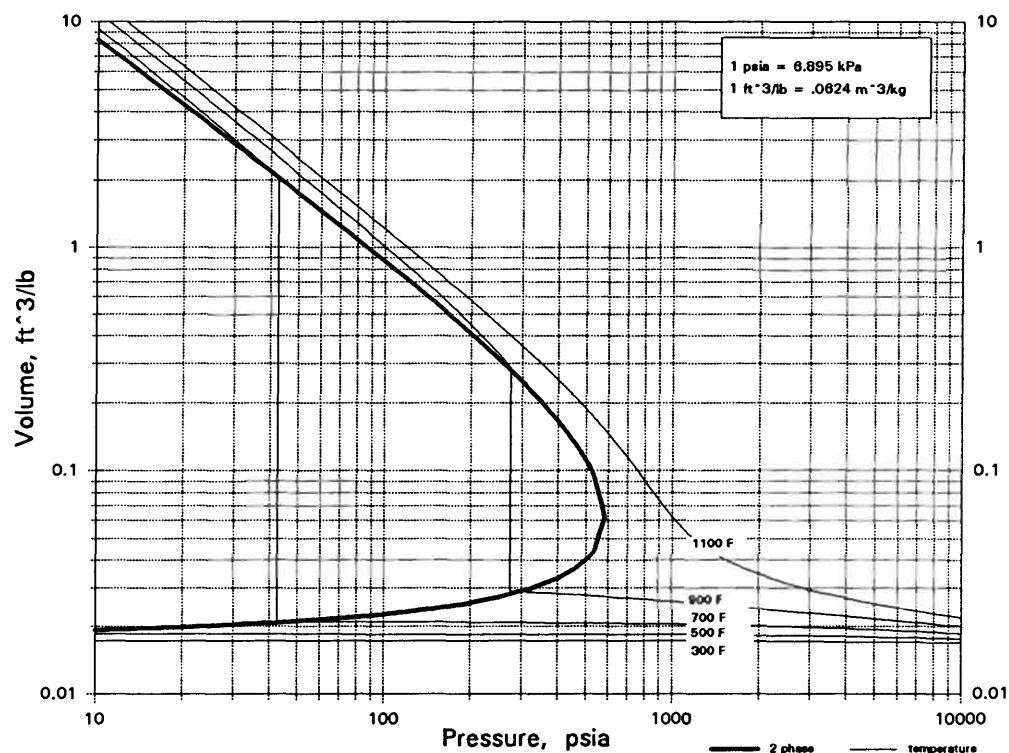
C5H8O3

METHYL ACETOACETATE



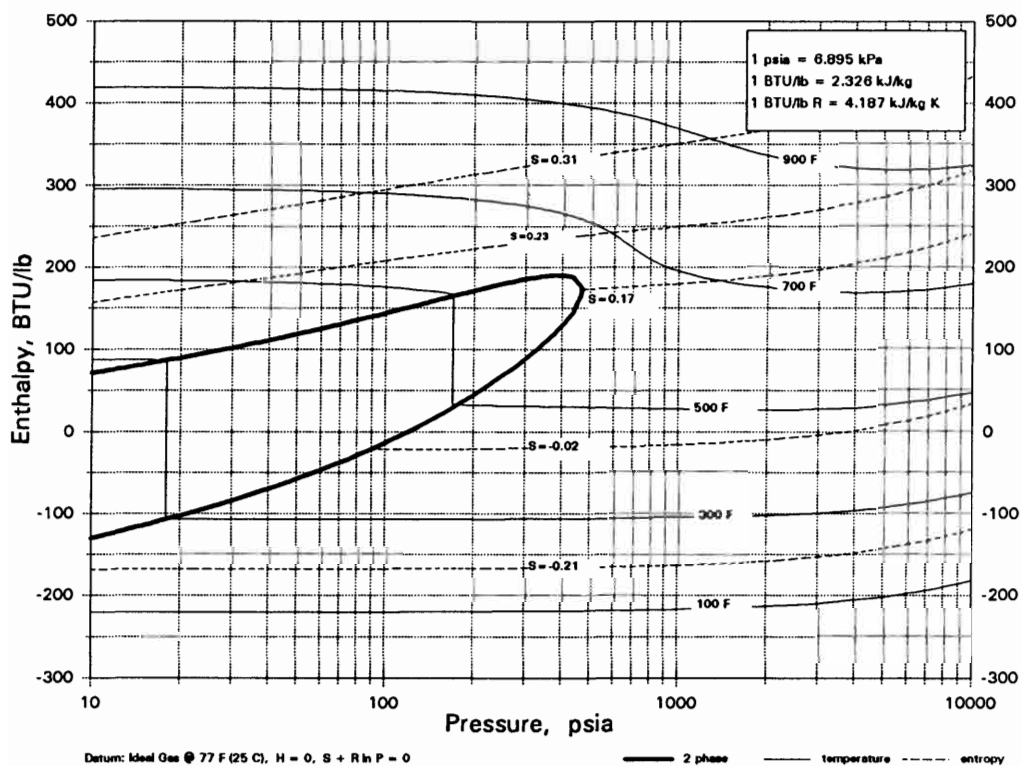
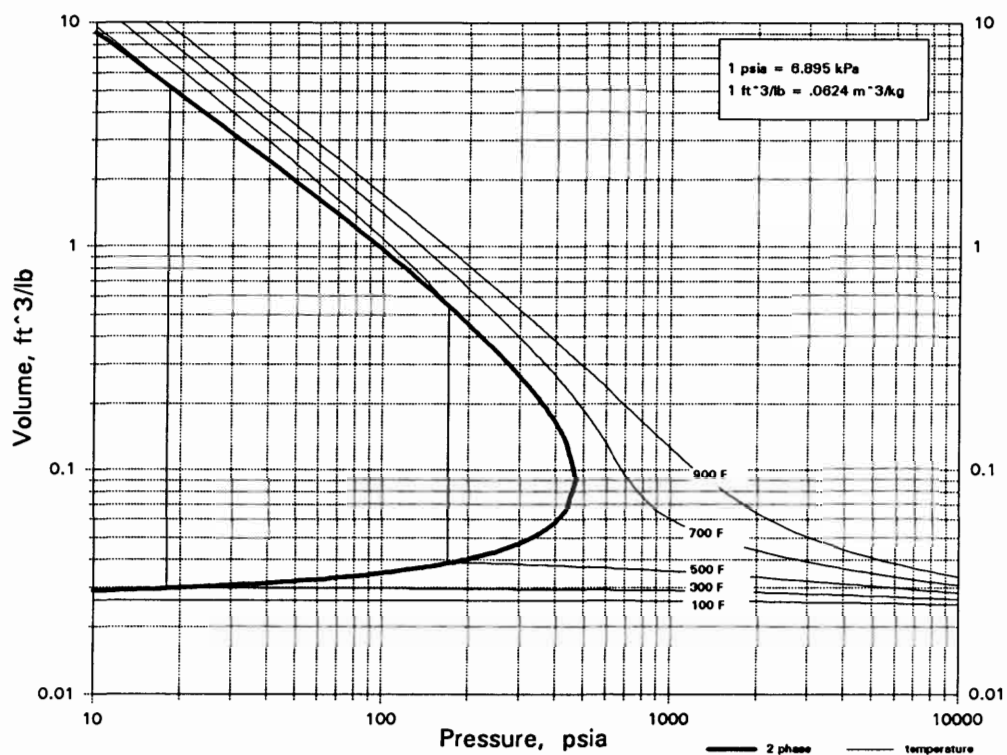
C5H8O4

GLUTARIC ACID



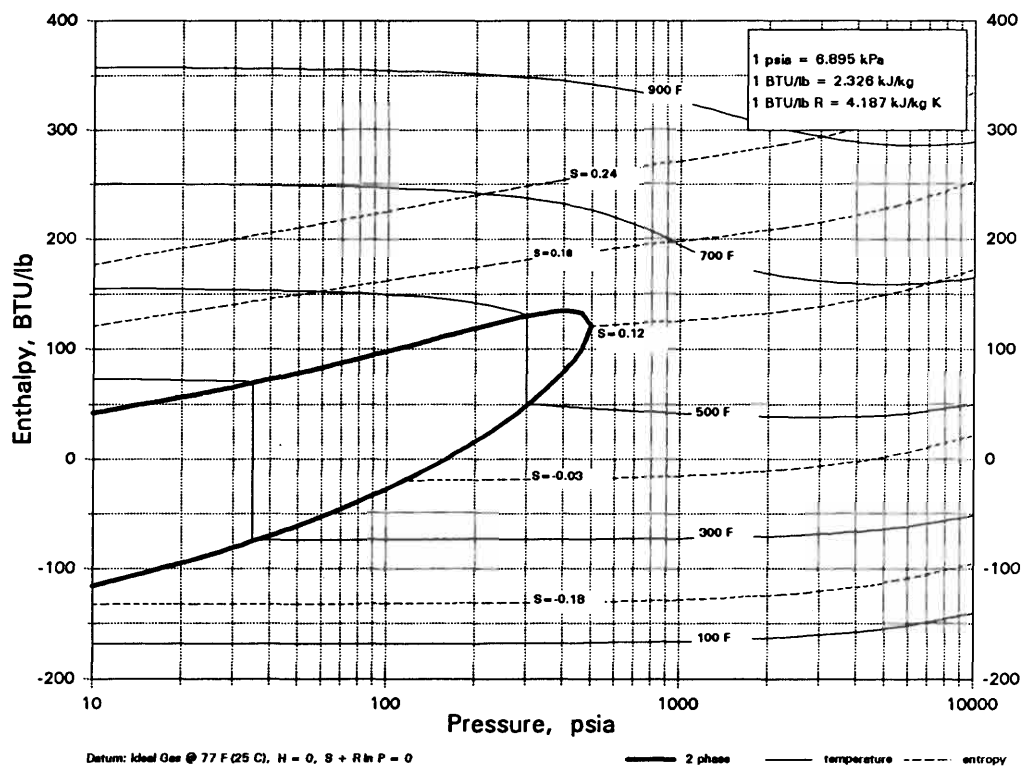
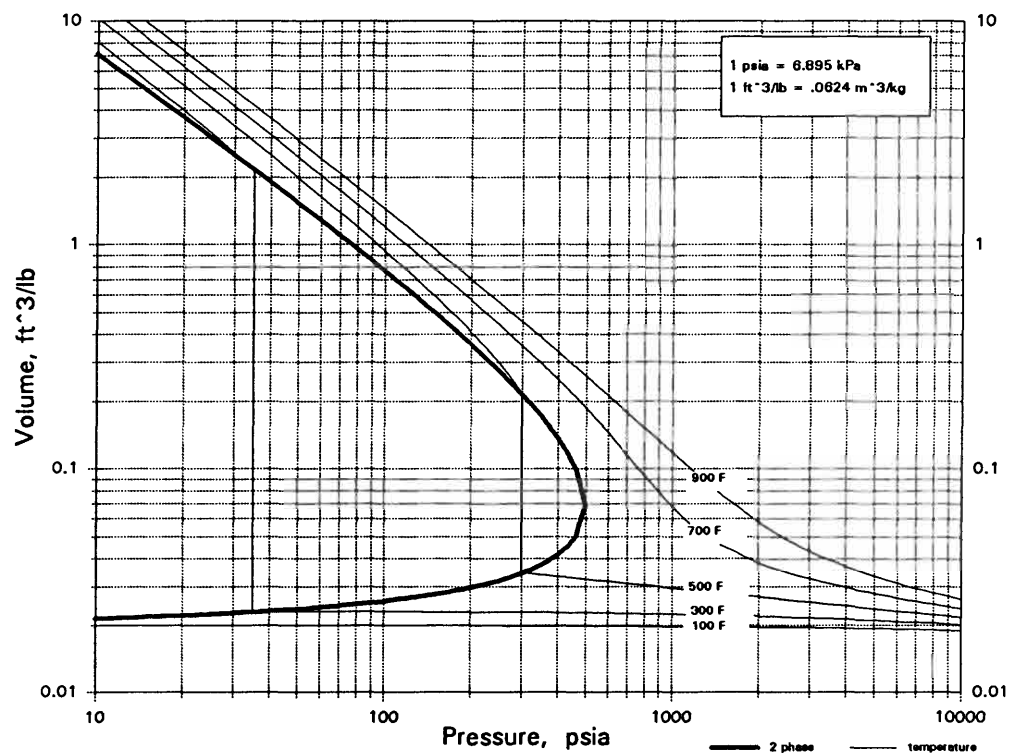
C5H9N

VALERONITRILE



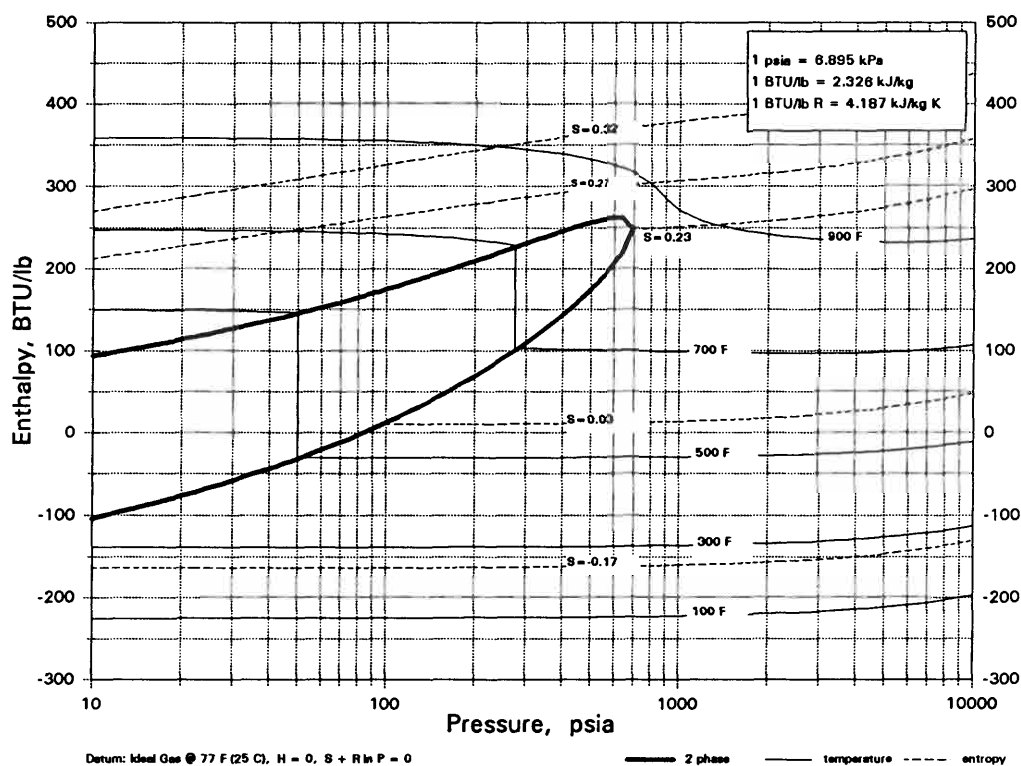
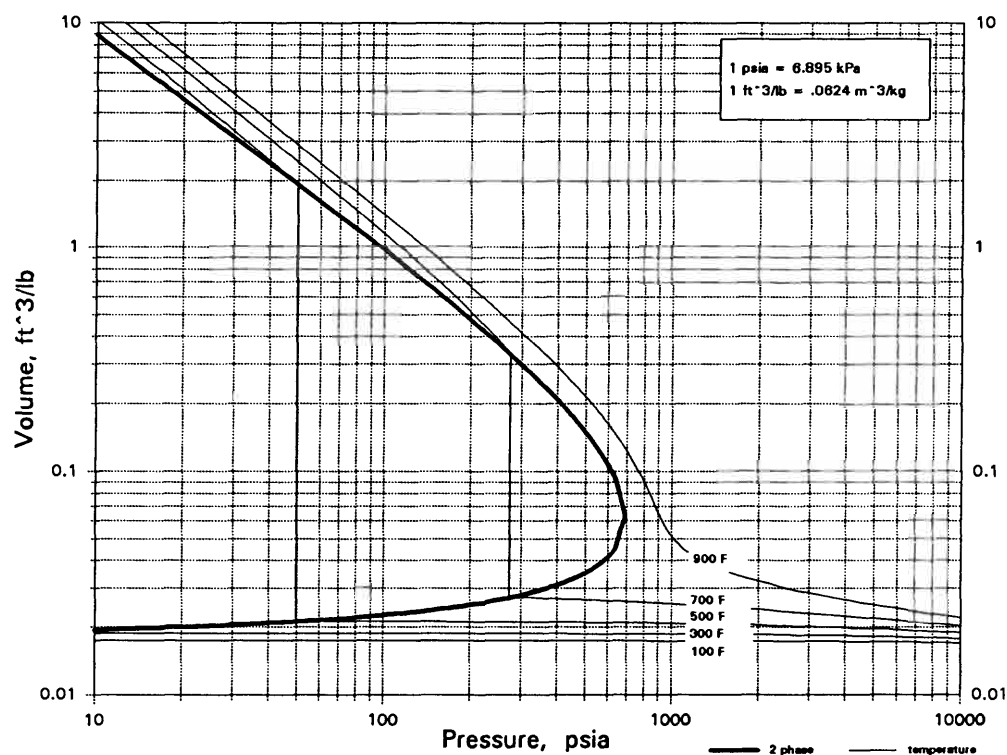
C₅H₉NO

n-BUTYL ISOCYANATE



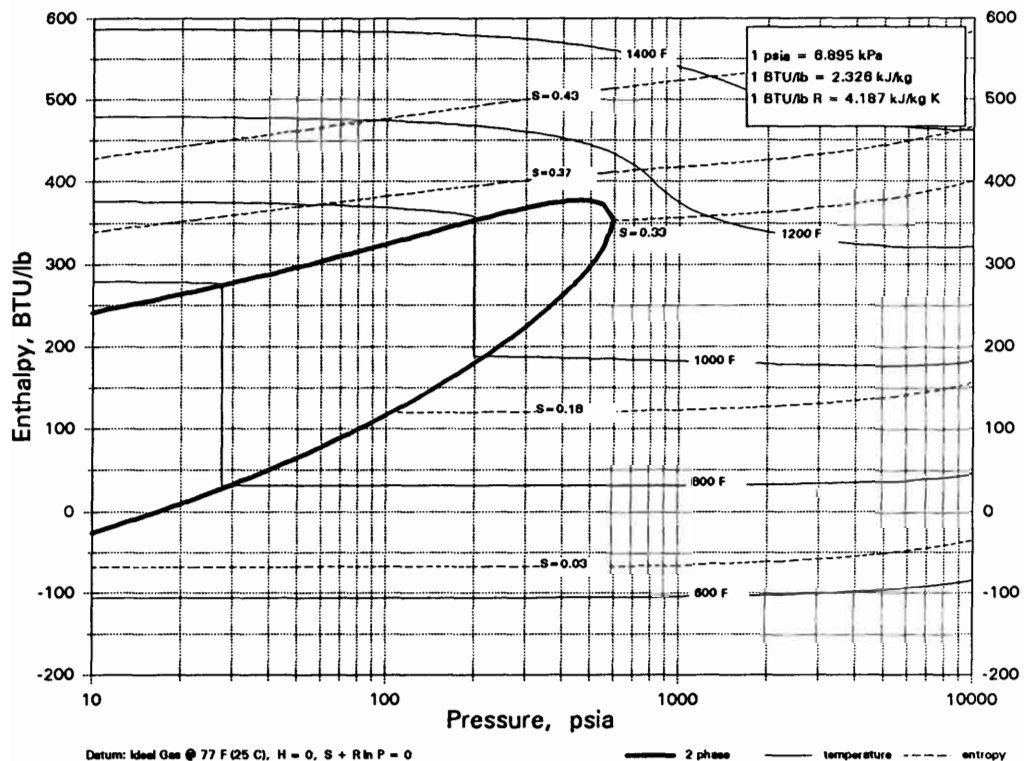
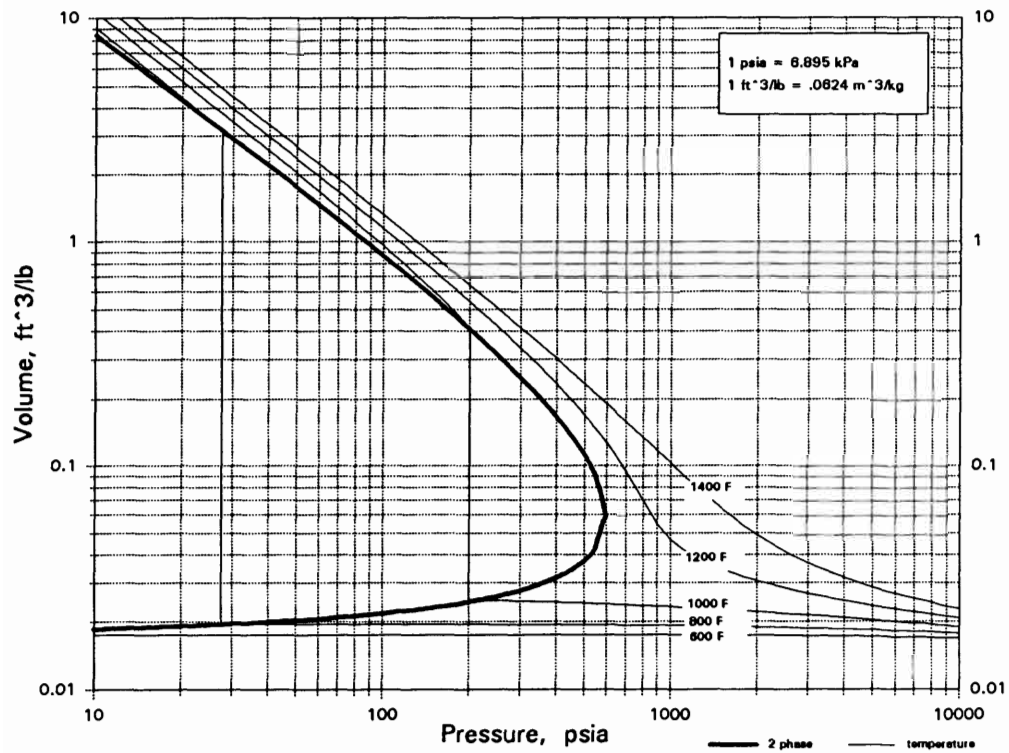
C5H9NO

N-METHYL-2-PYRROLIDONE

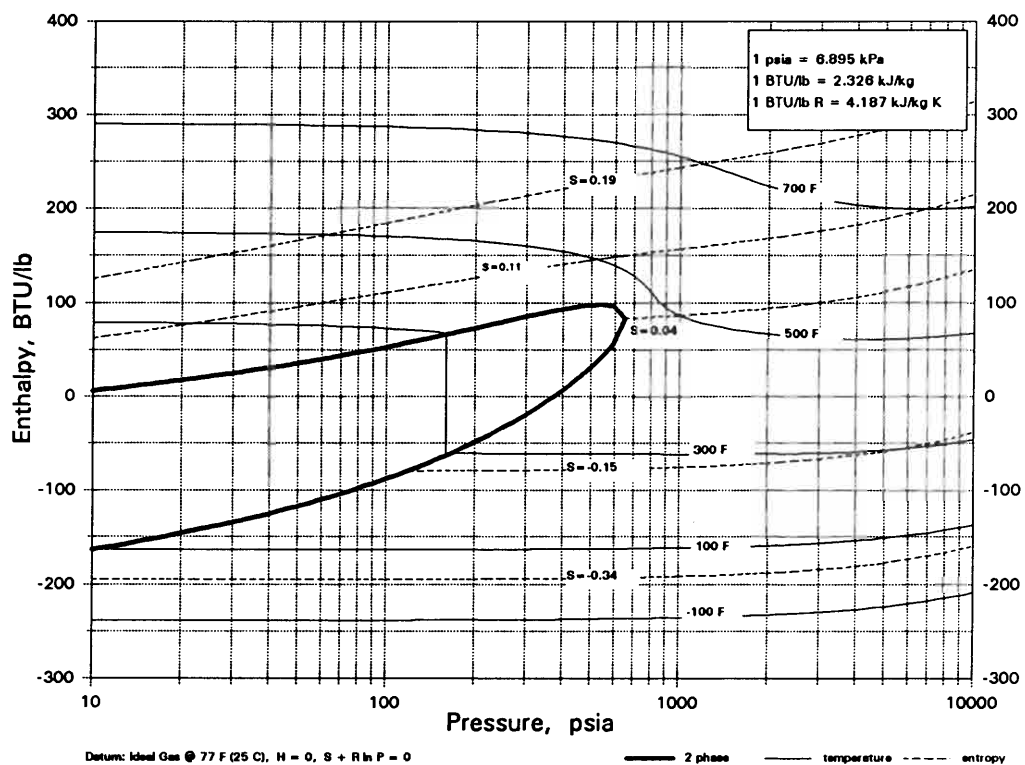
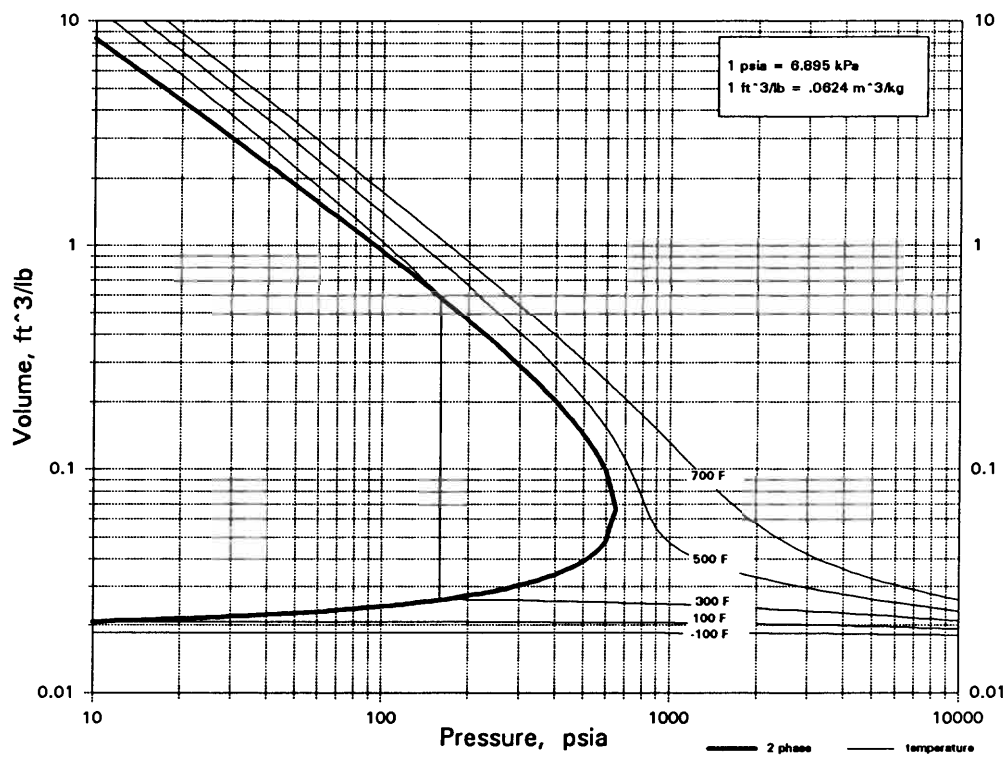


C5H9NO4

L-GLUTAMIC ACID

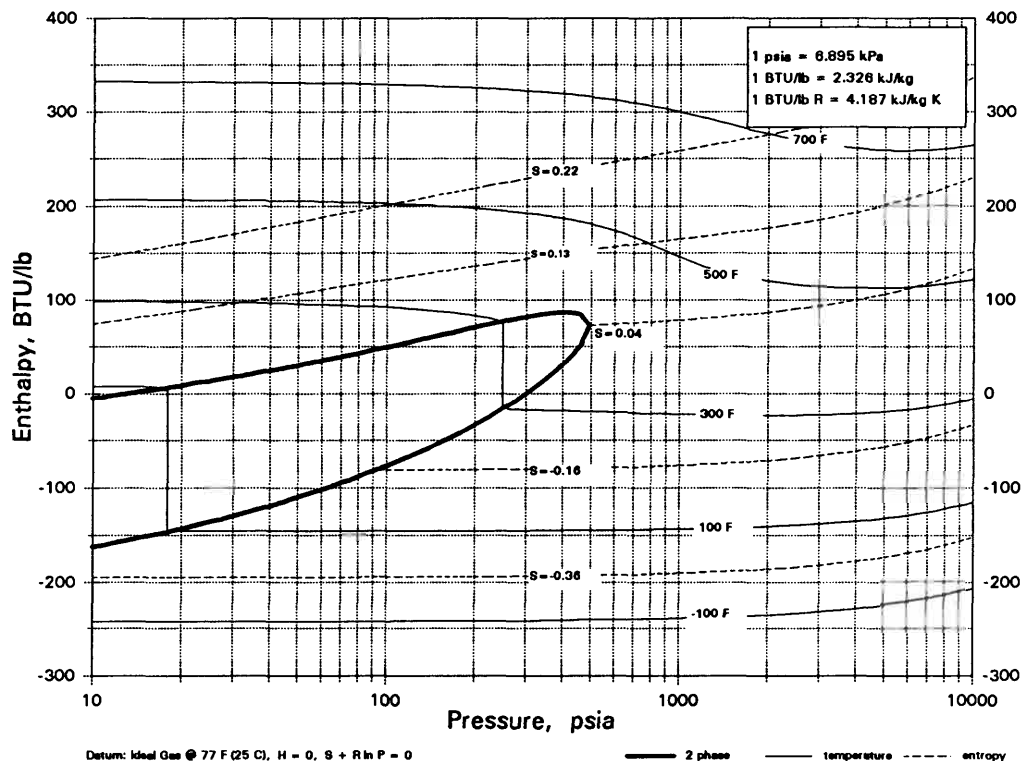
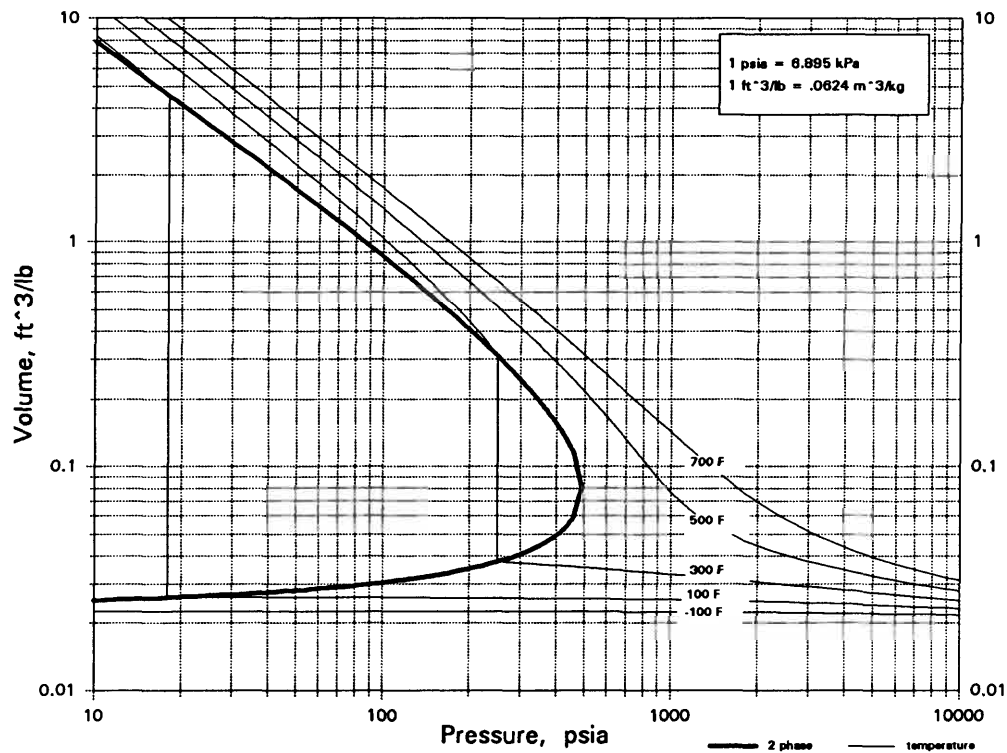


C5H10
CYCLOPENTANE



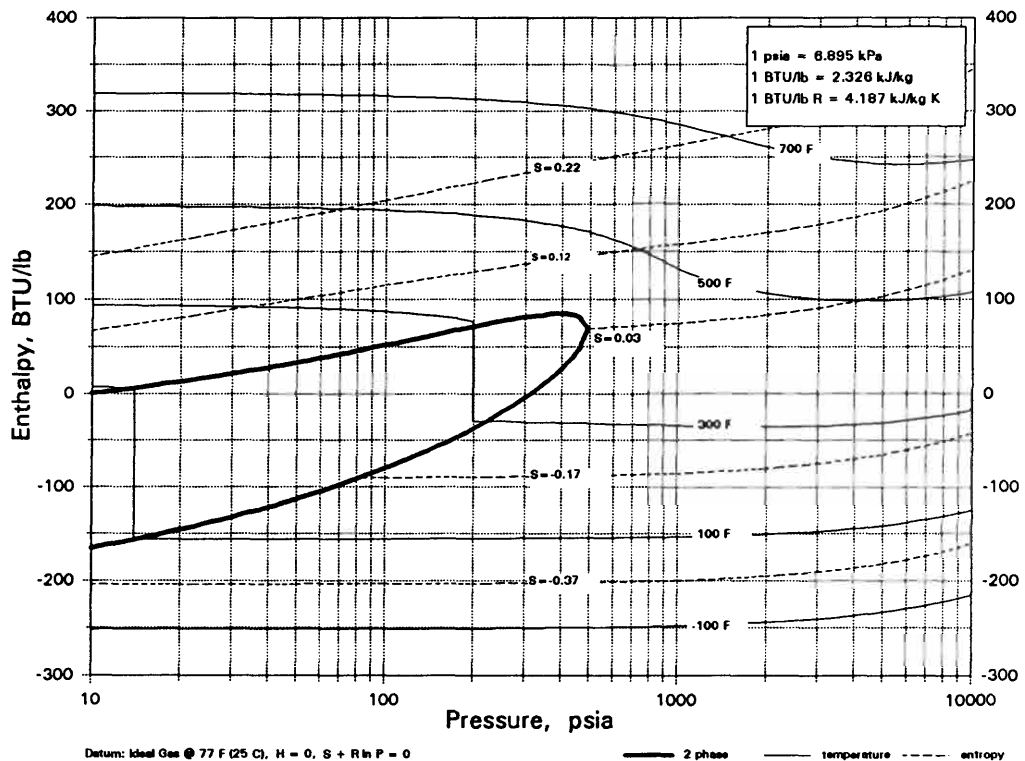
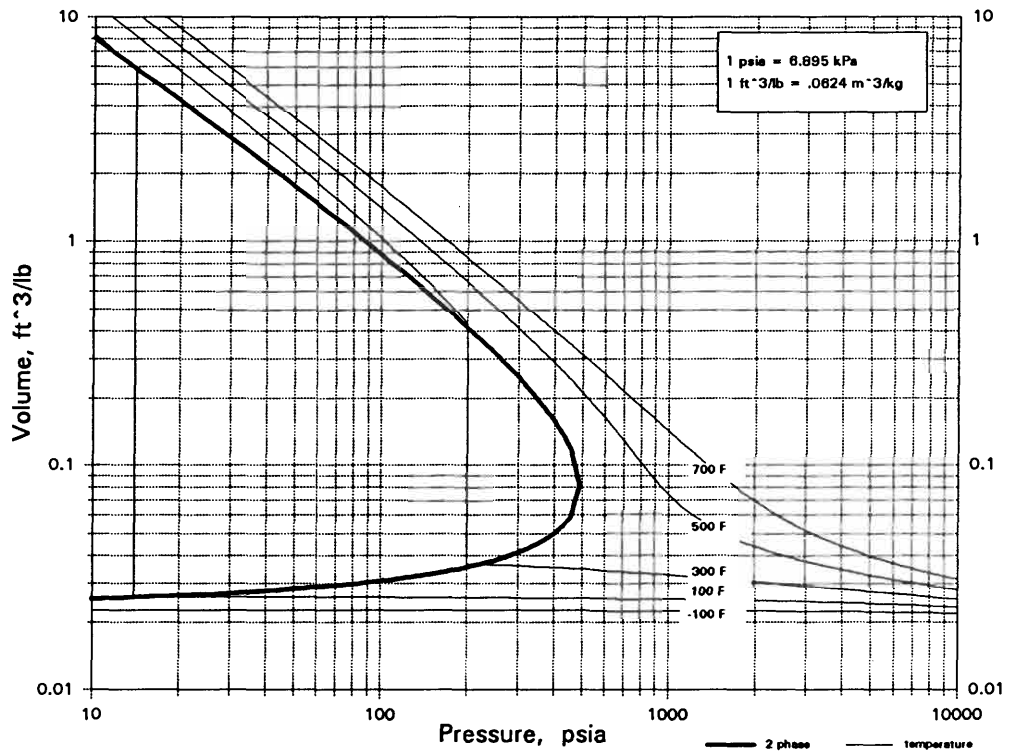
C5H10

2-METHYL-1-BUTENE



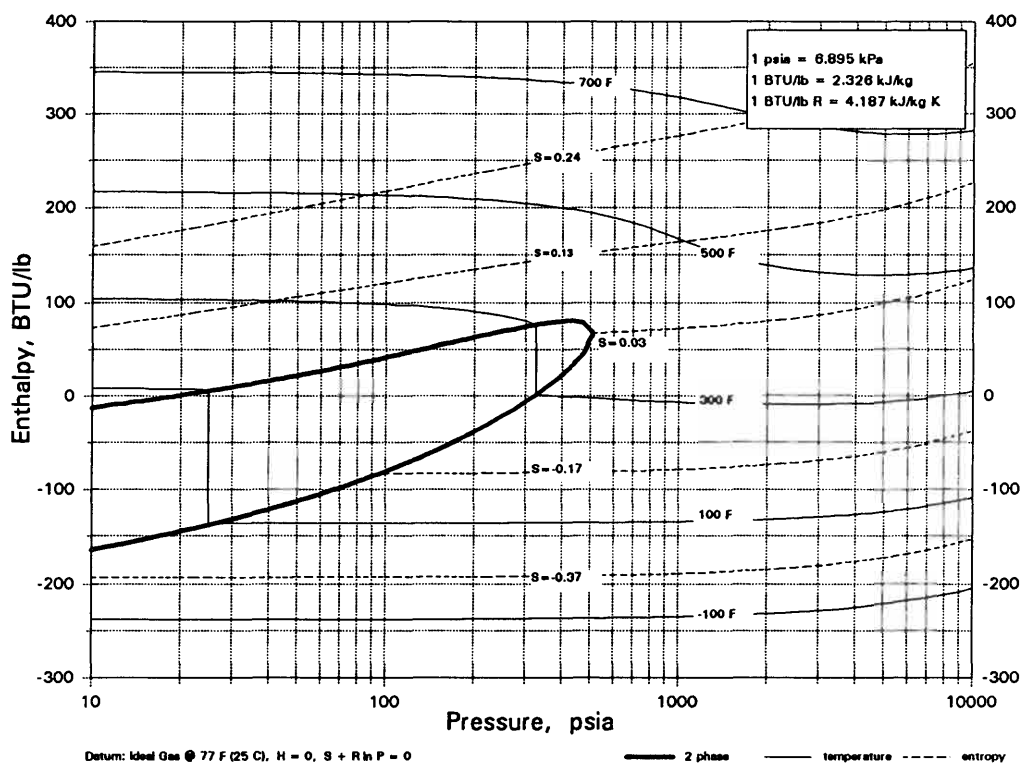
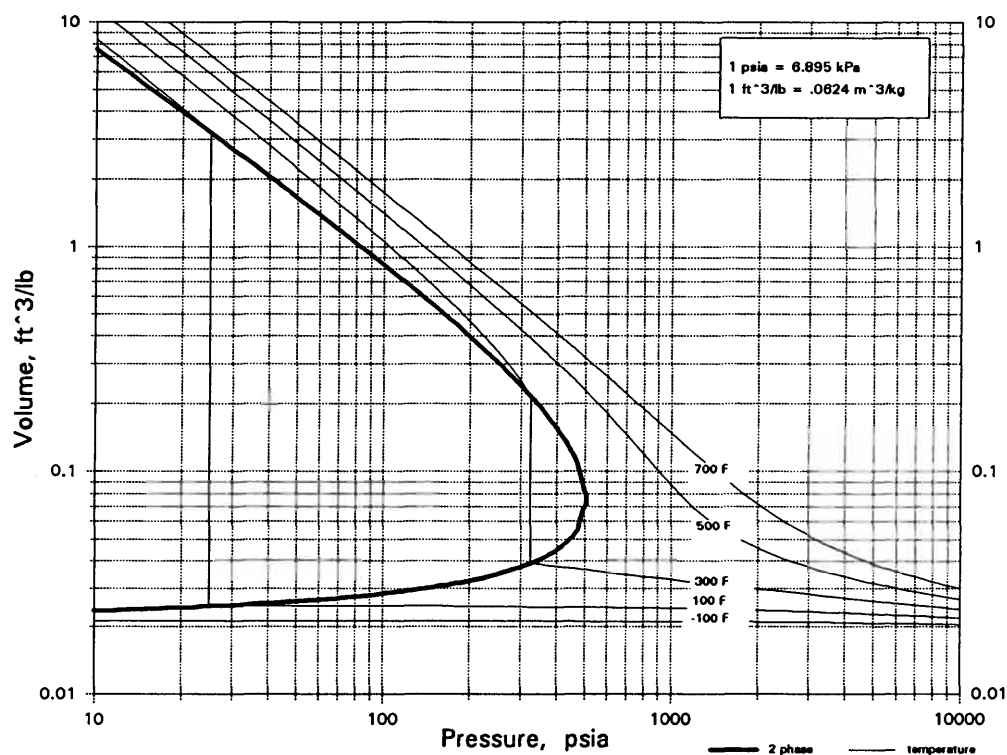
C5H10

2-METHYL-2-BUTENE



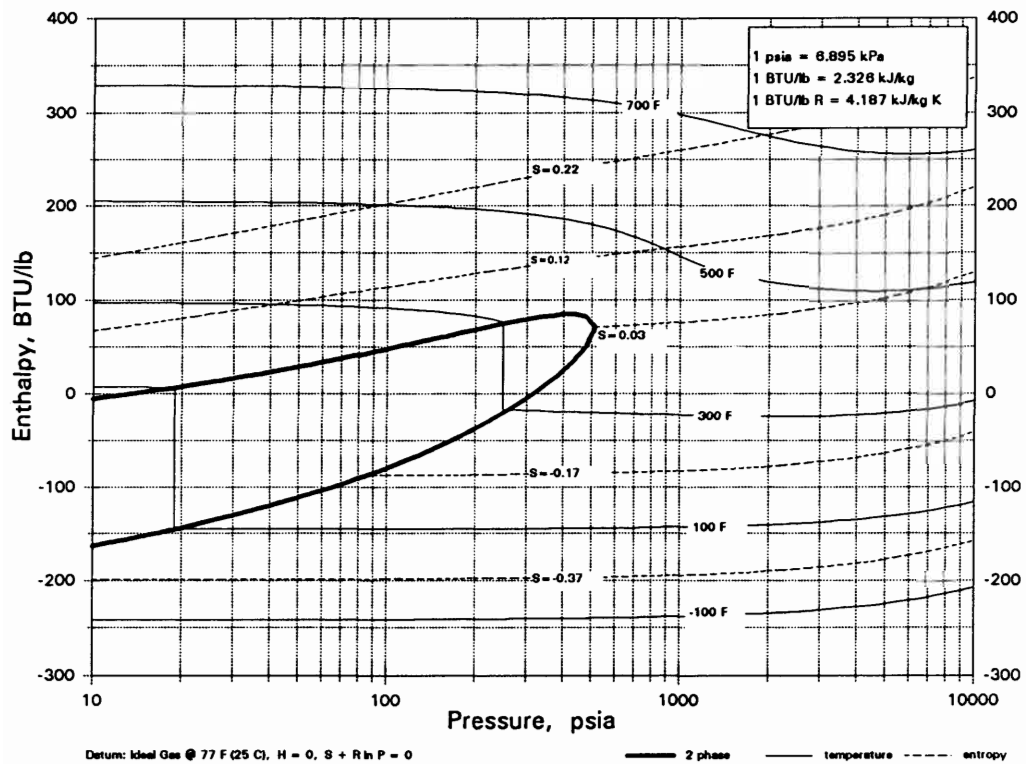
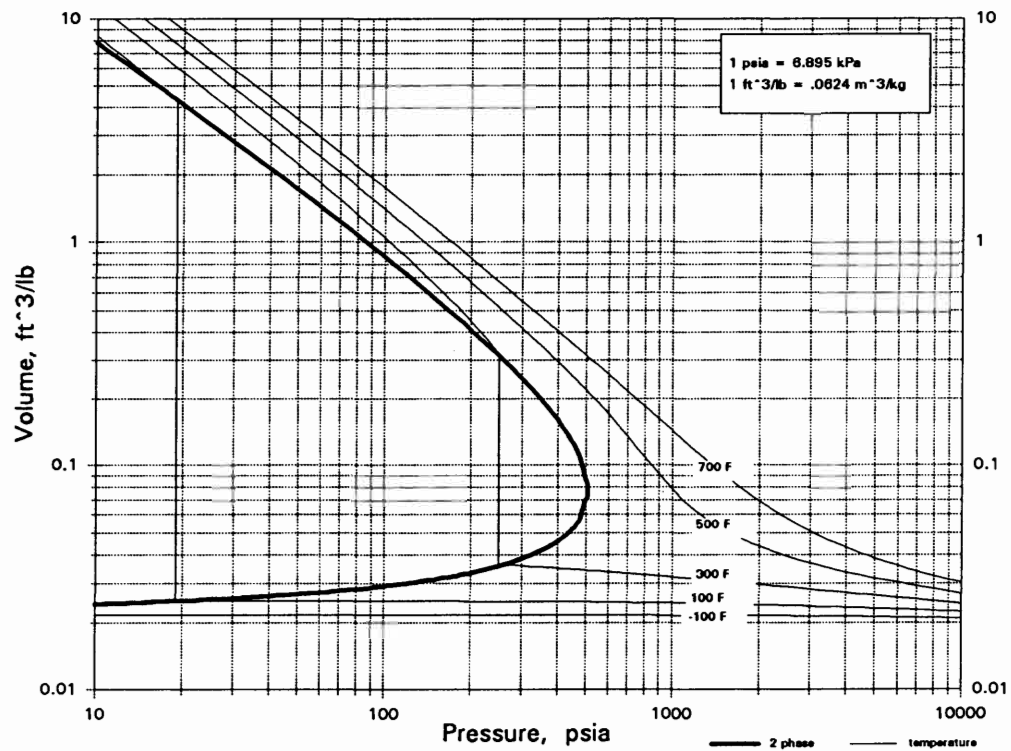
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3-METHYL-1-BUTENE



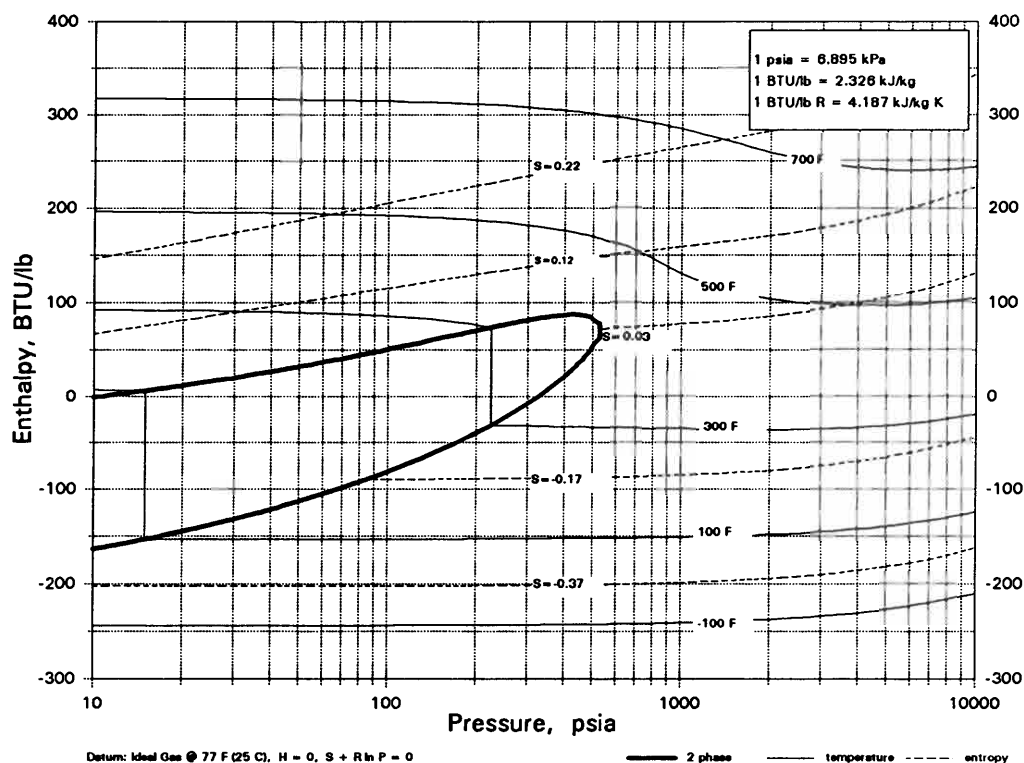
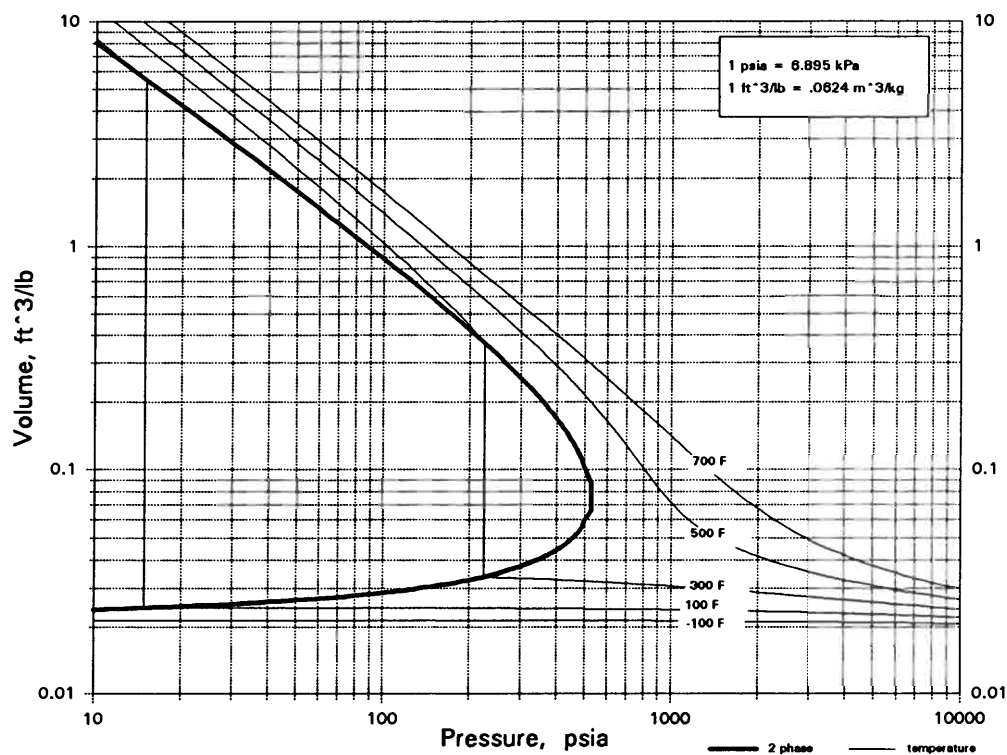
C5H10

1-PENTENE



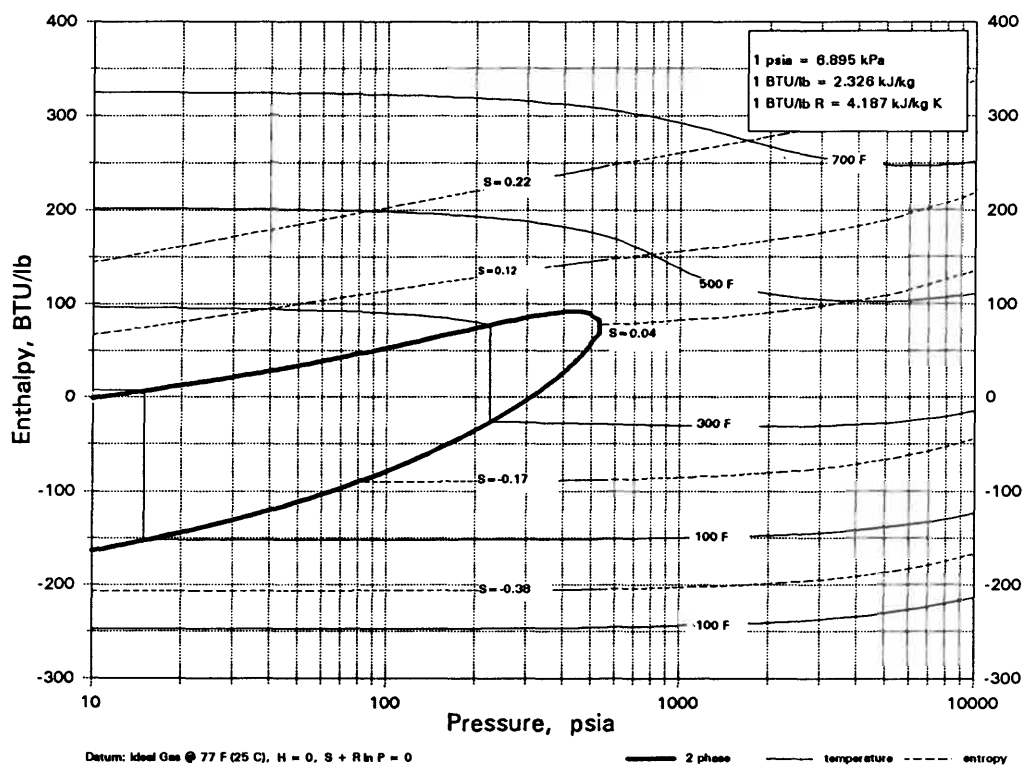
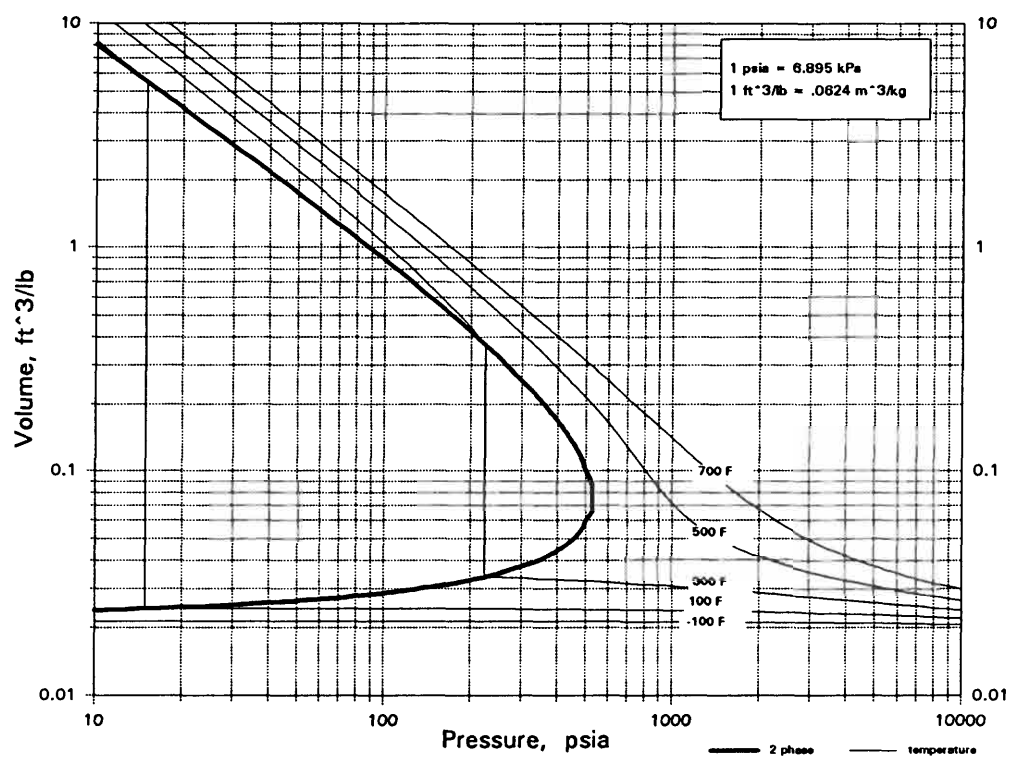
C5H10

cis-2-PENTENE



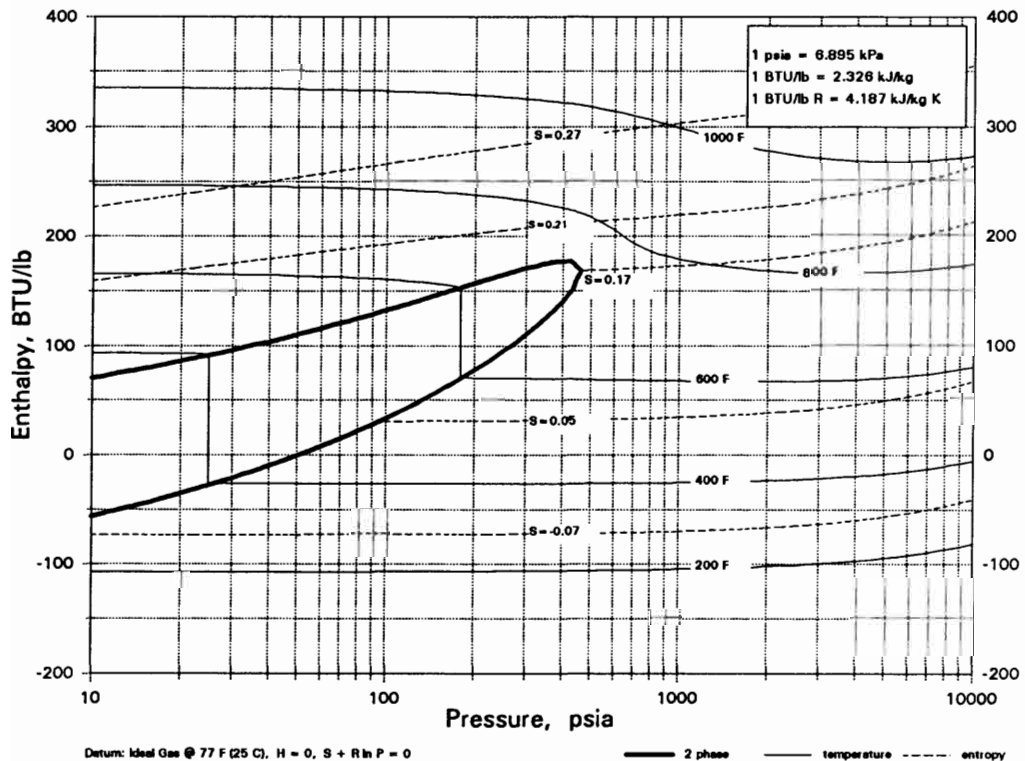
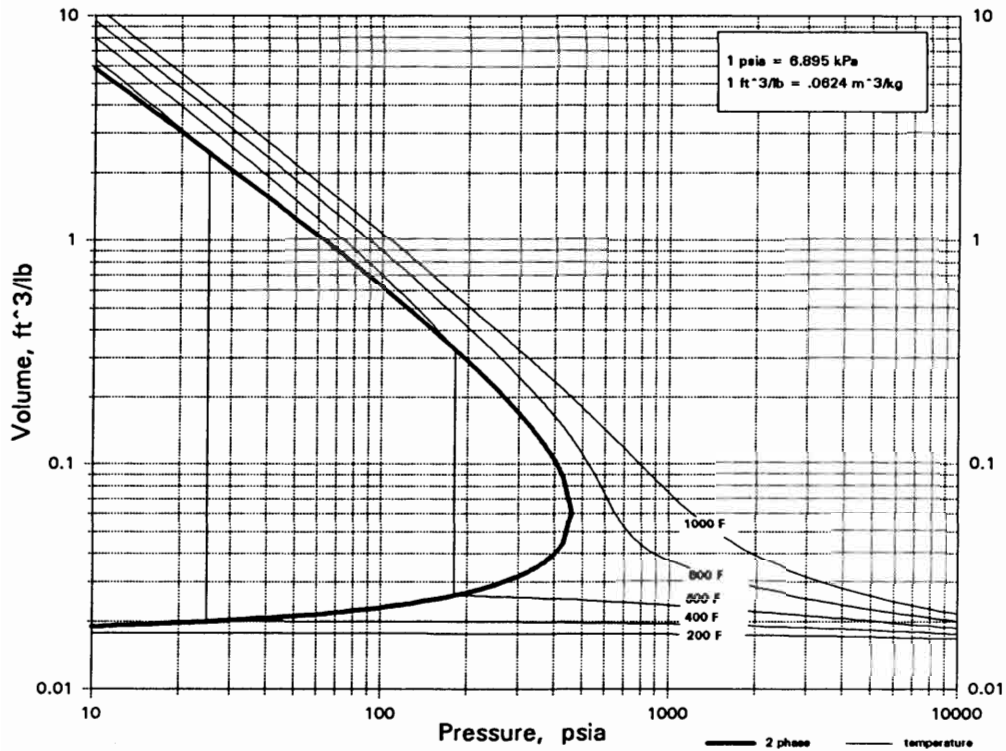
C5H10

trans-2-PENTENE



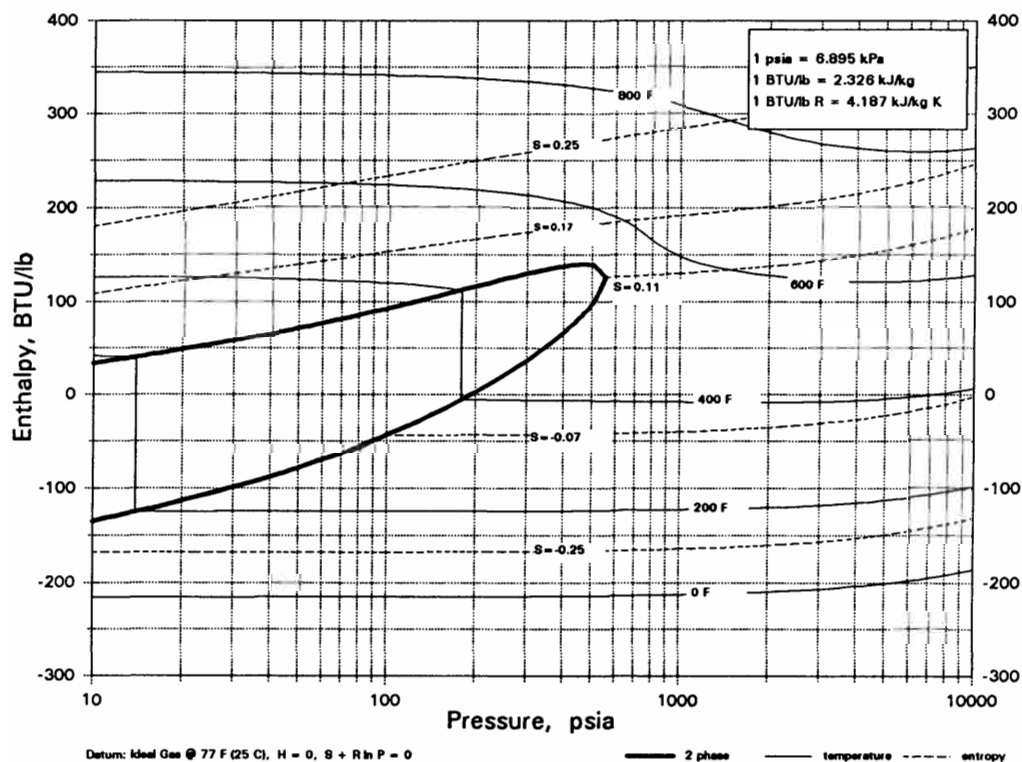
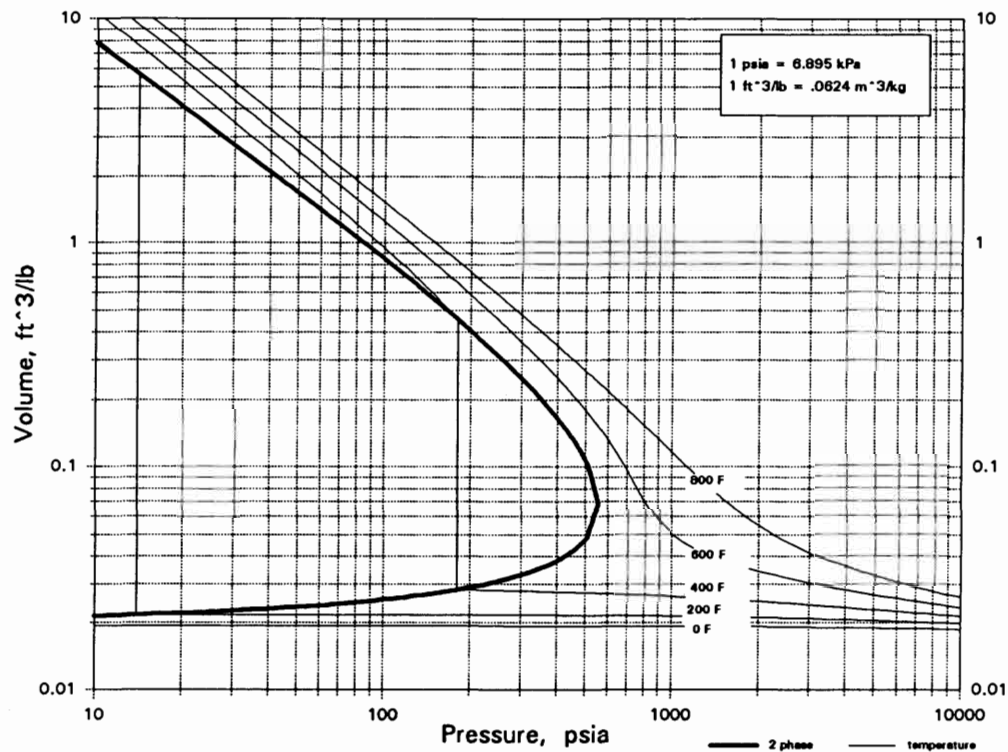
C₅H₁₀Cl₂

1-5-DICHLOROPENTANE



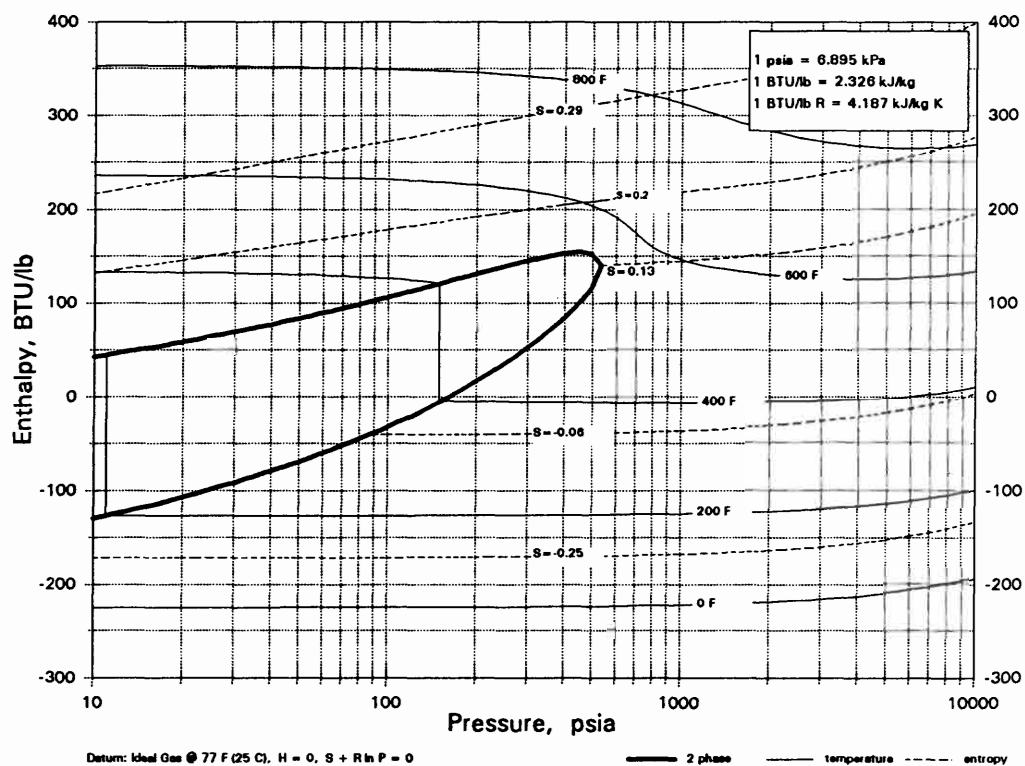
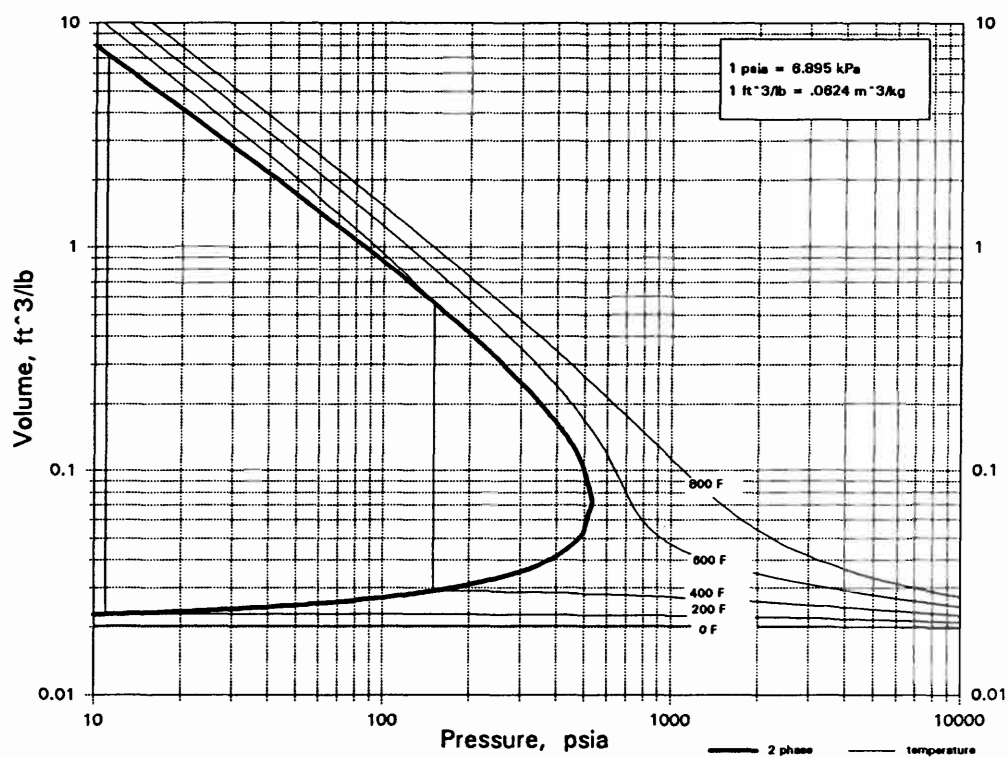
C5H10O

METHYL ISOPROPYL KETONE



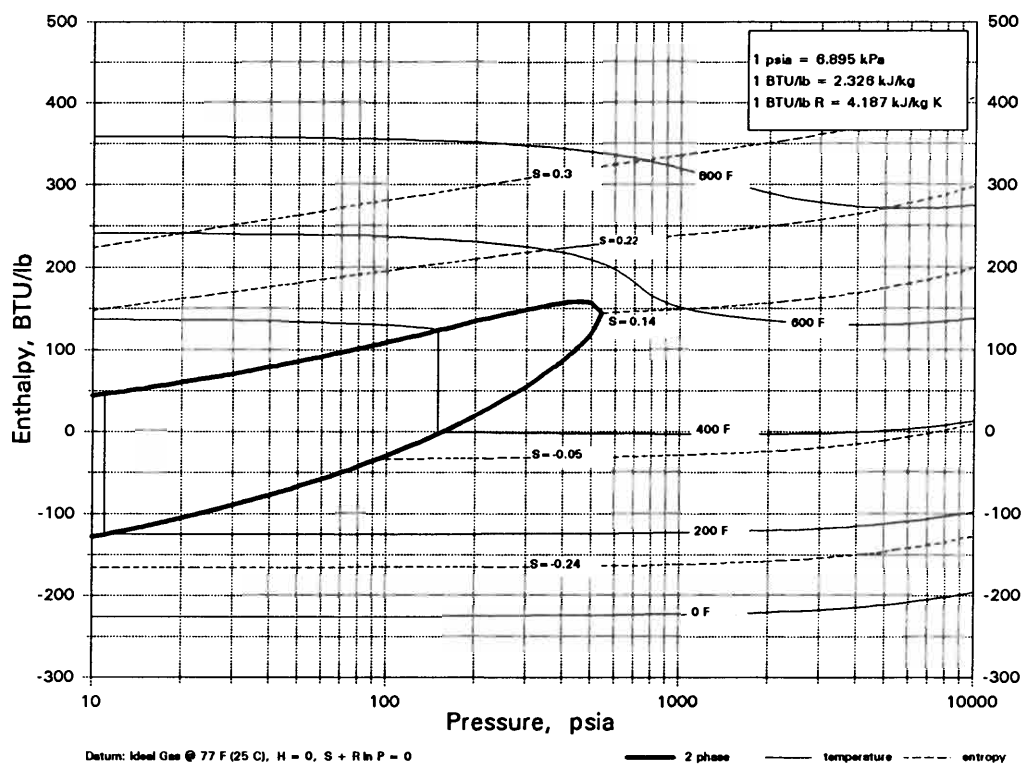
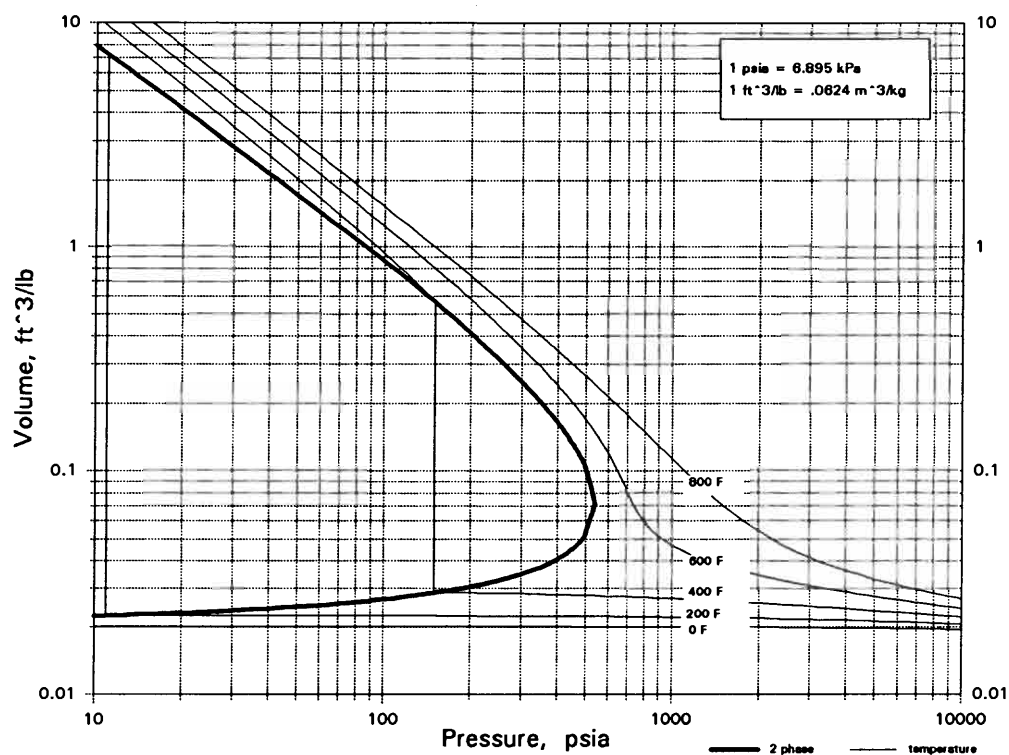
C5H10O

2-PENTANONE



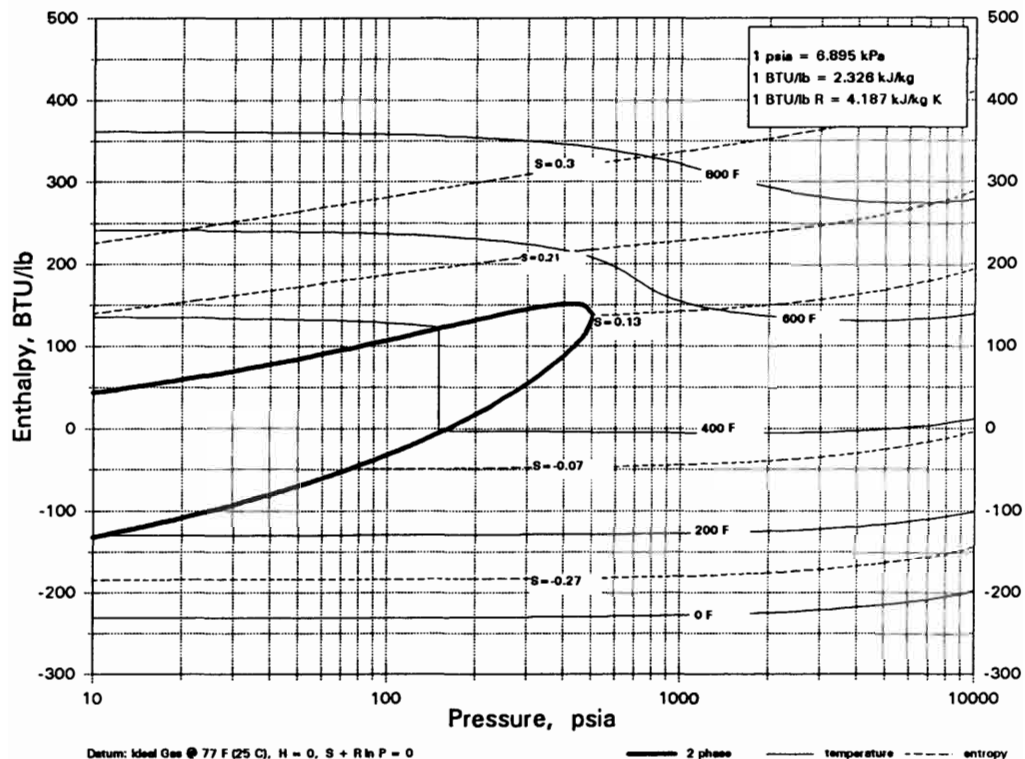
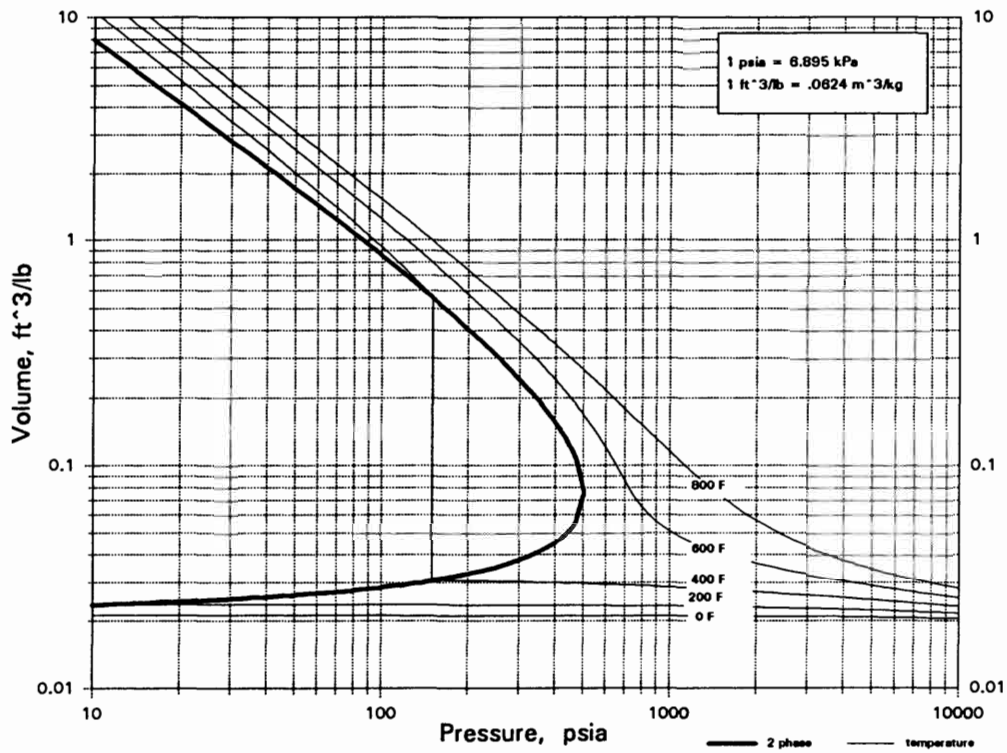
C5H10O

DIETHYL KETONE



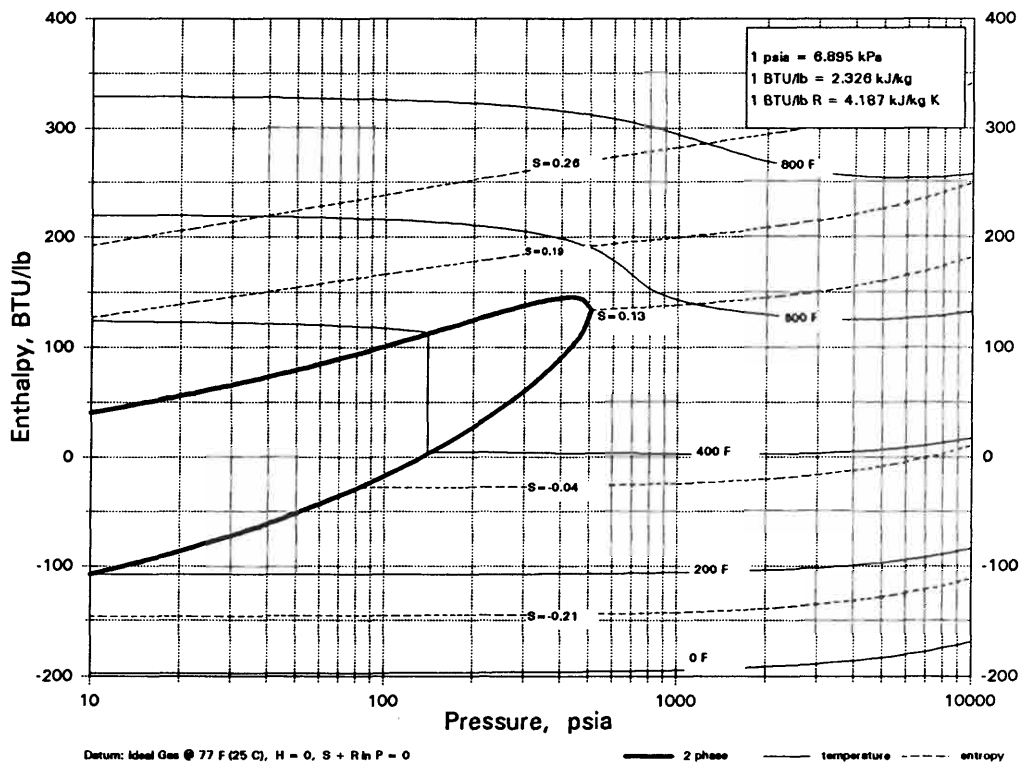
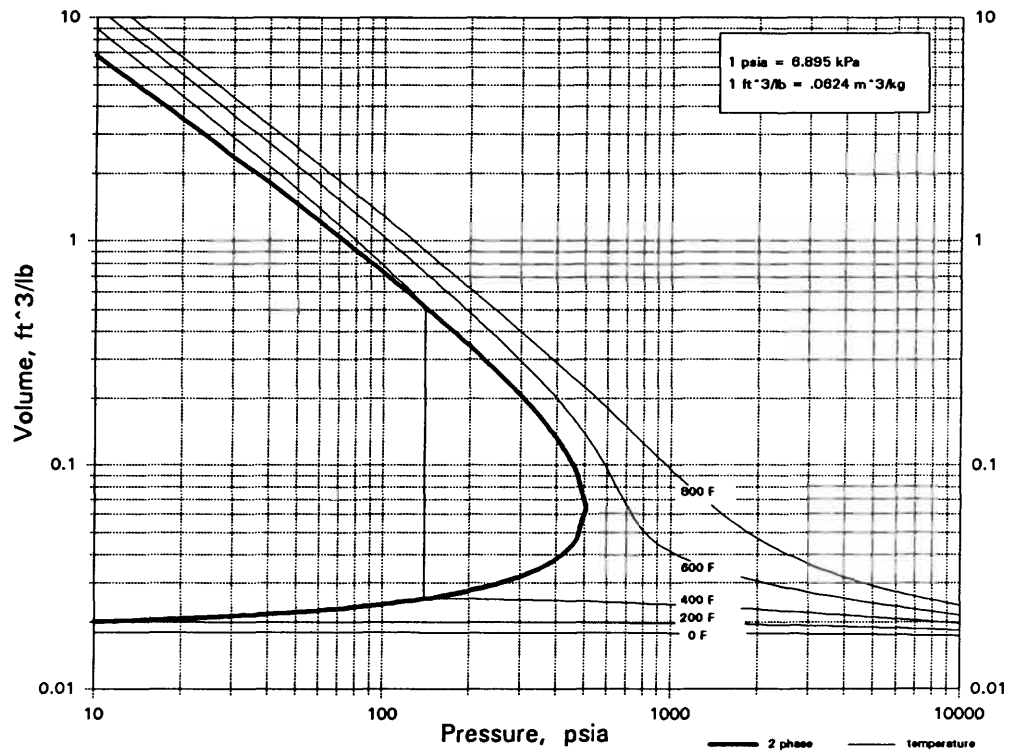
C5H10O

VALERALDEHYDE



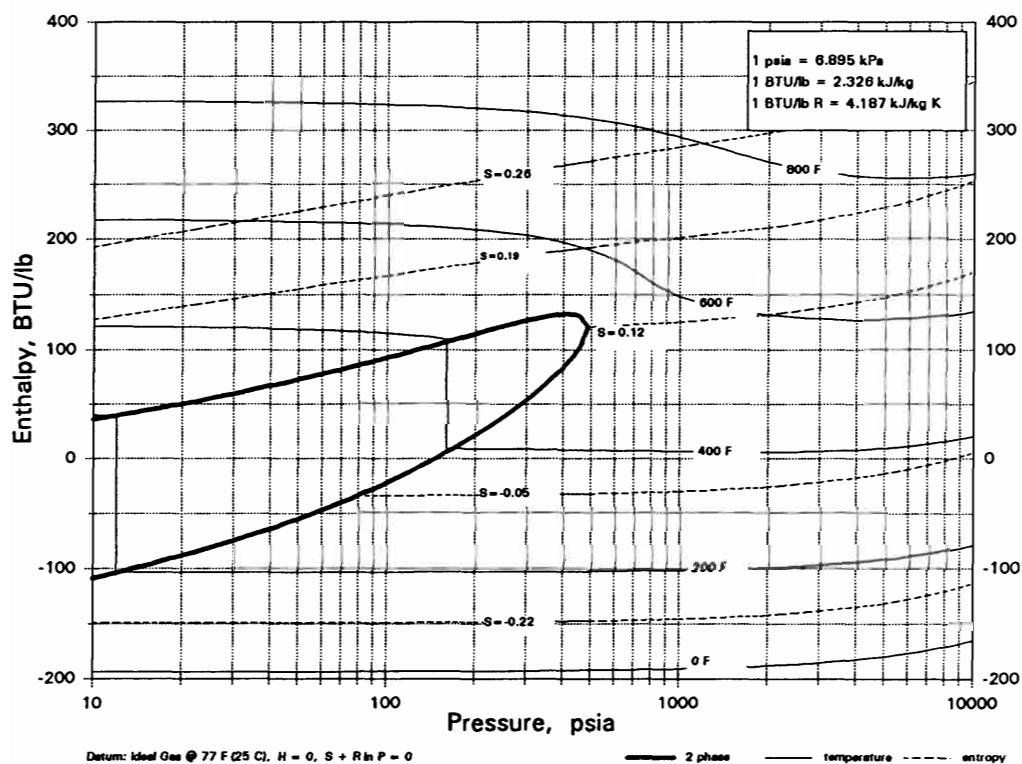
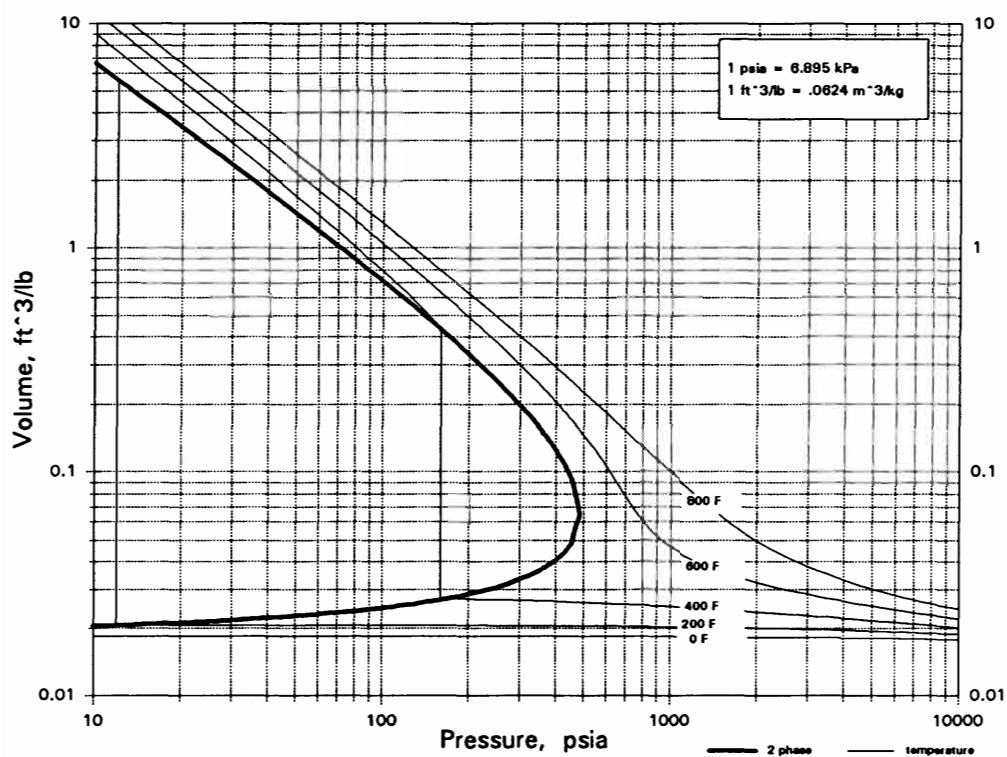
C5H10O2

n-BUTYL FORMATE



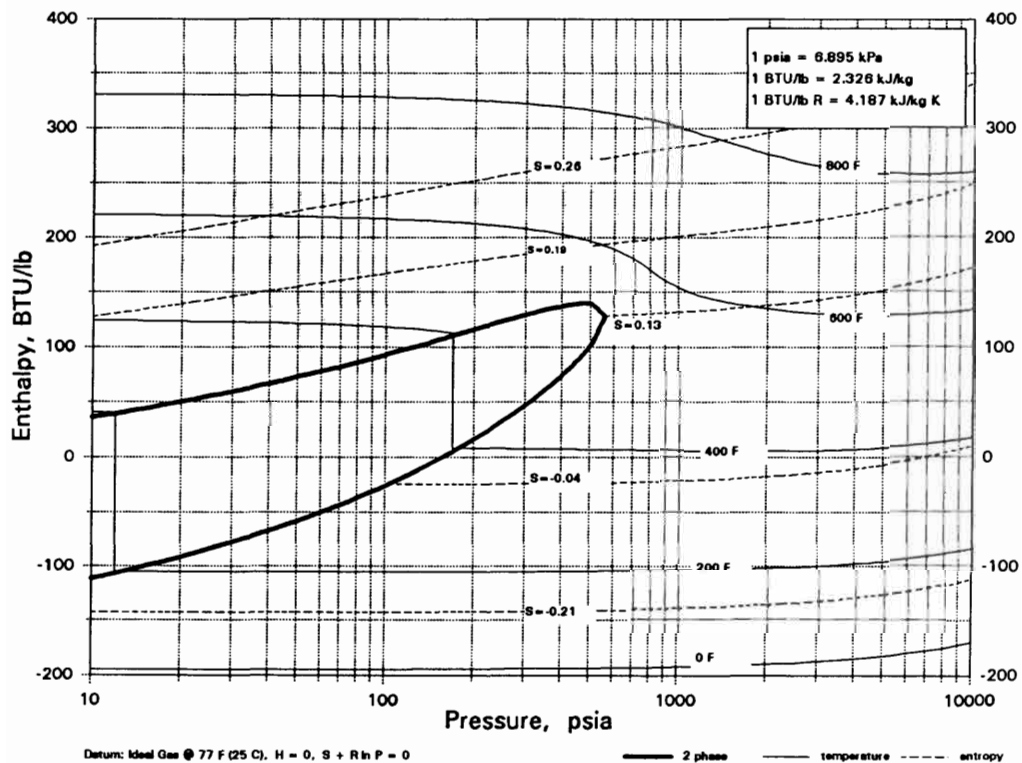
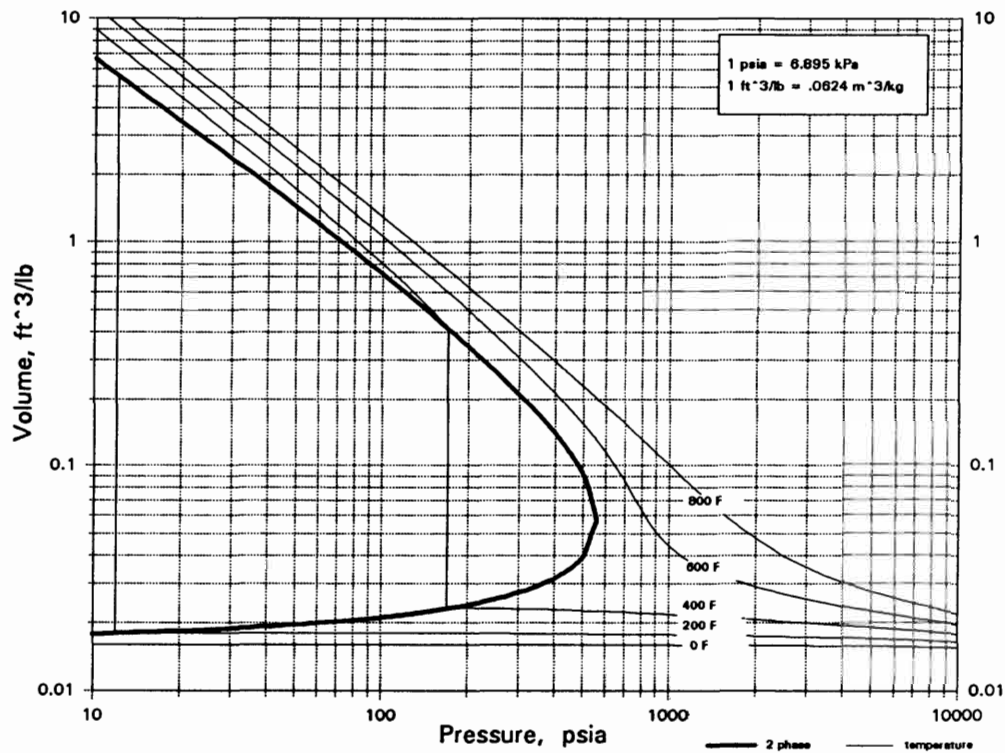
C5H10O2

ETHYL PROPIONATE



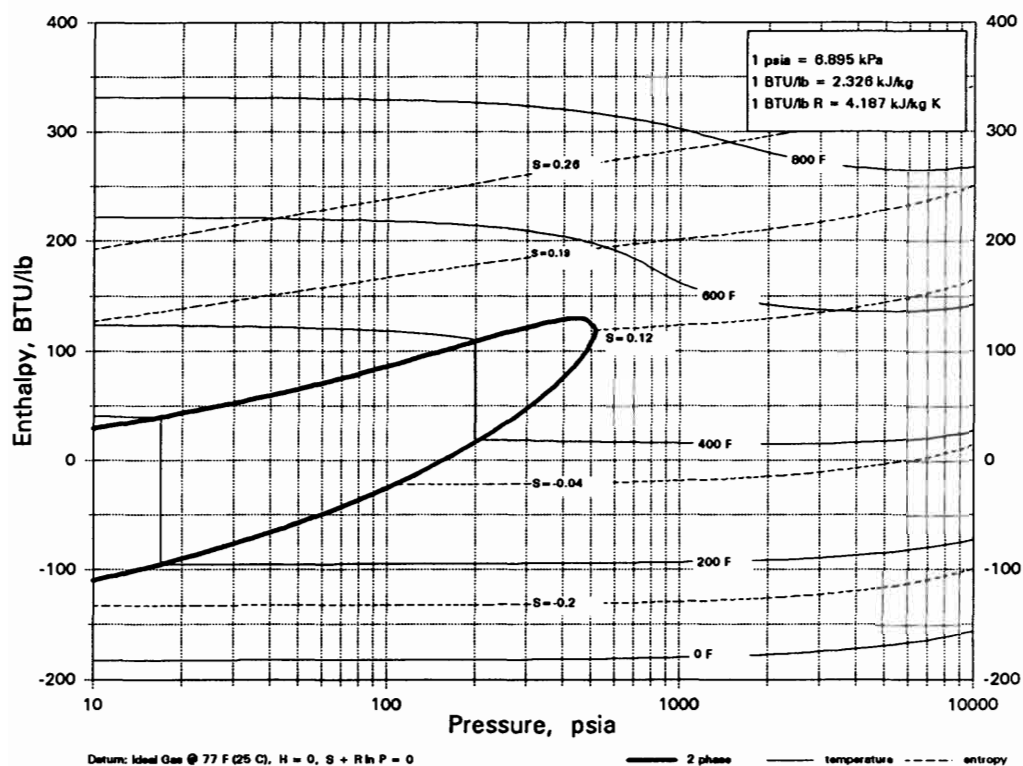
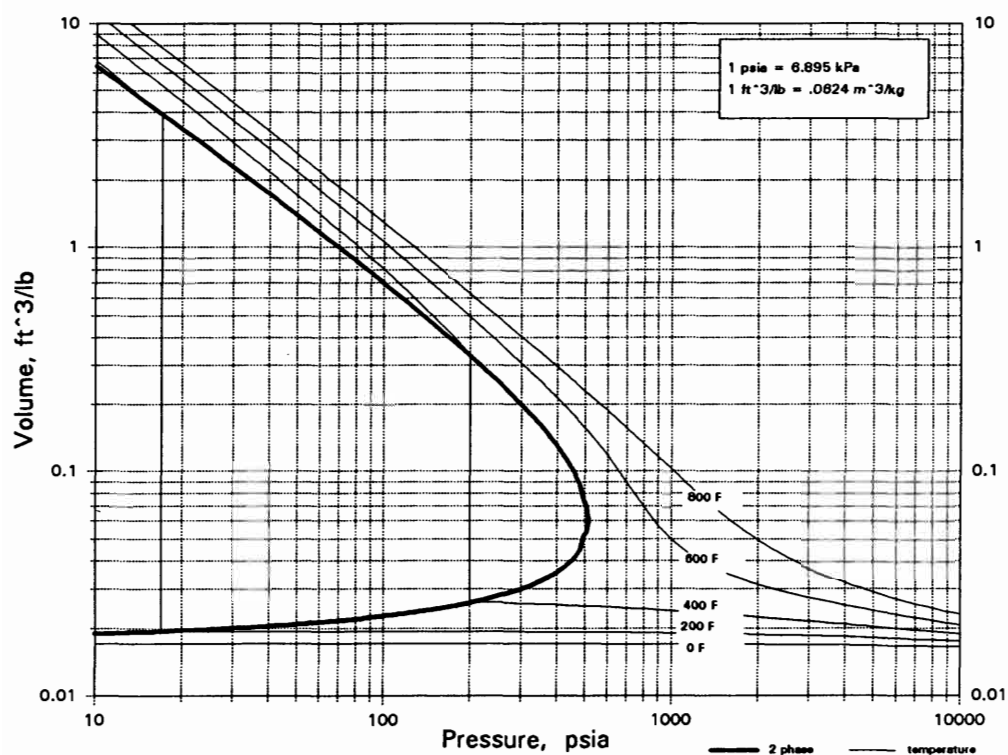
C5H10O2

ISOBUTYL FORMATE



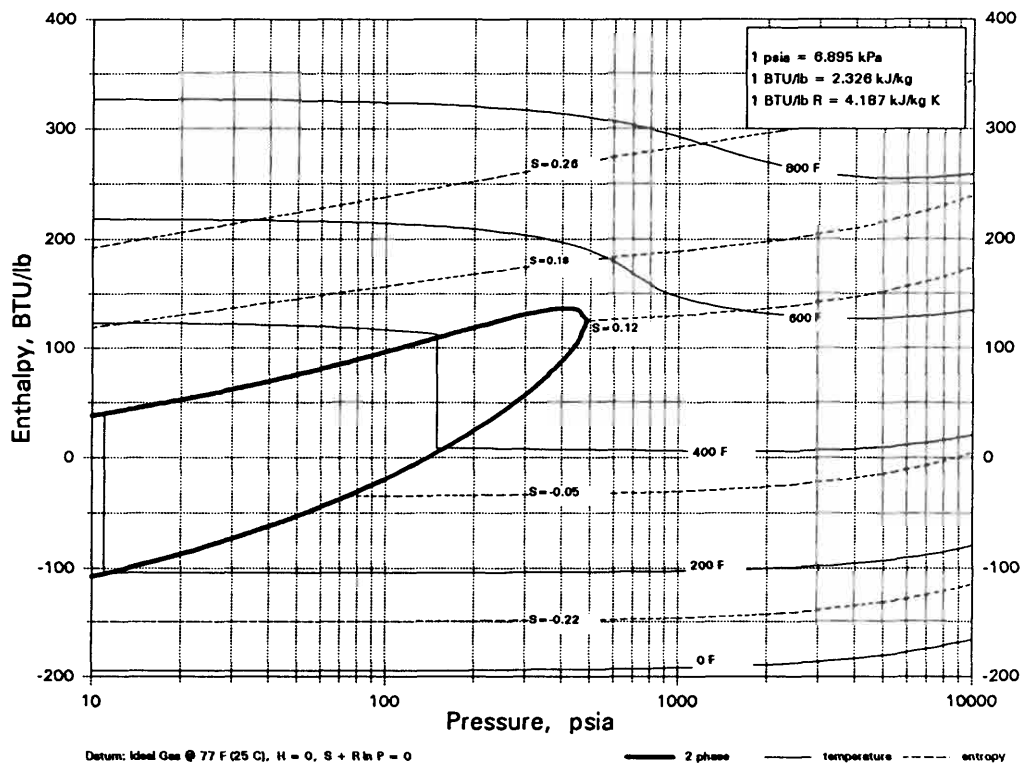
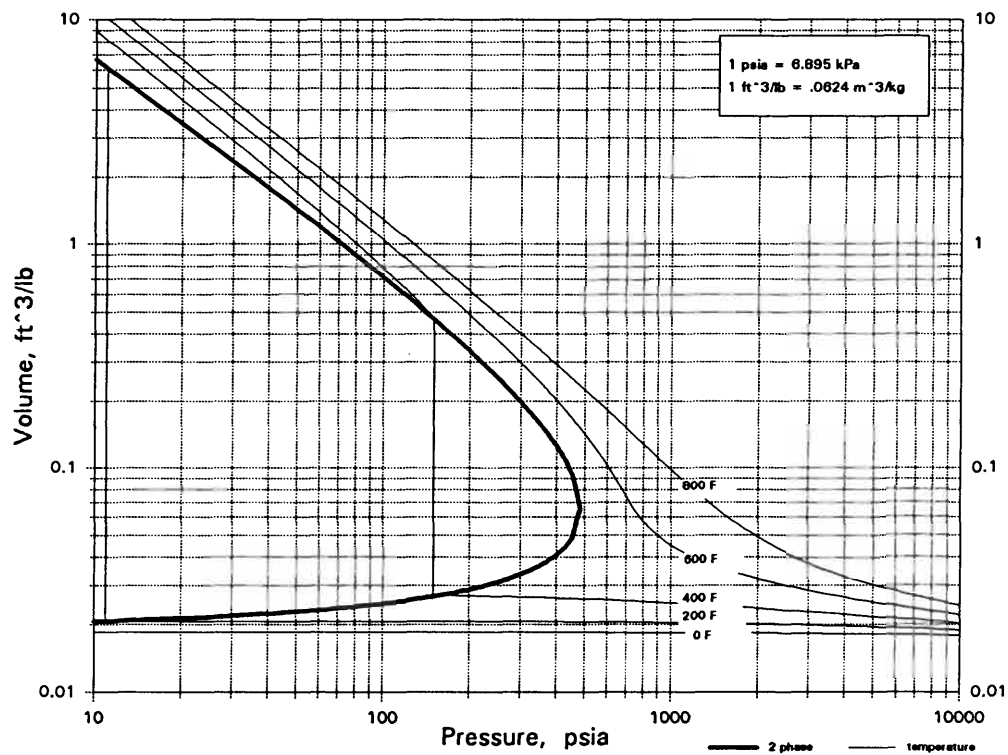
C5H10O2

ISOPROPYL ACETATE



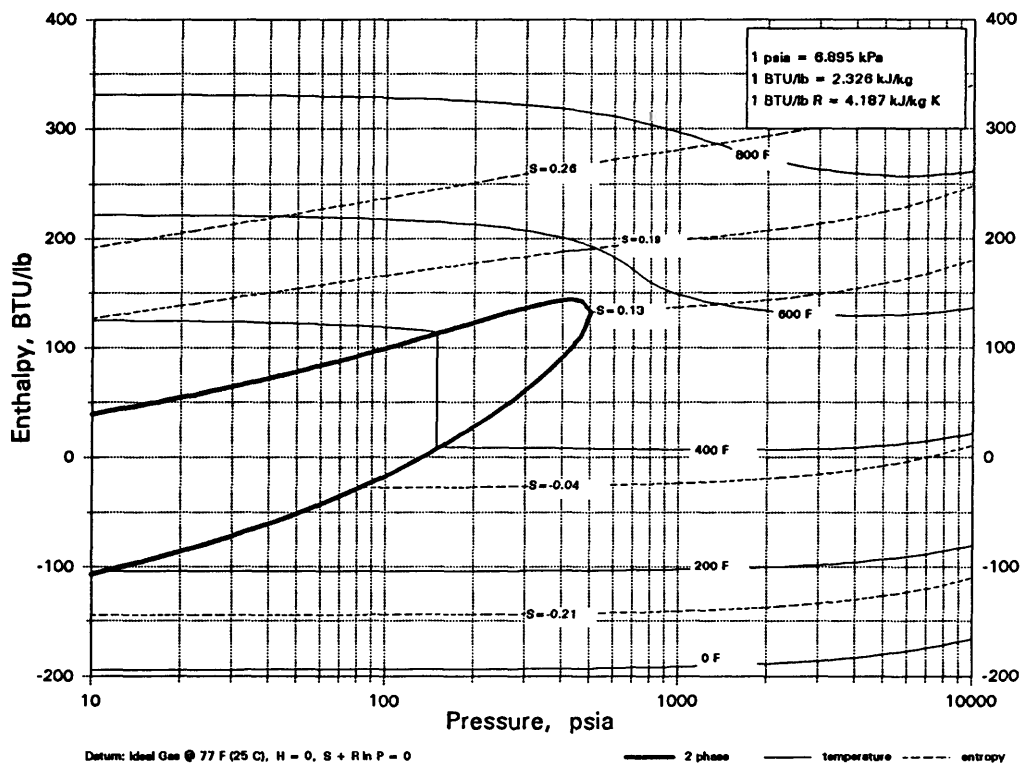
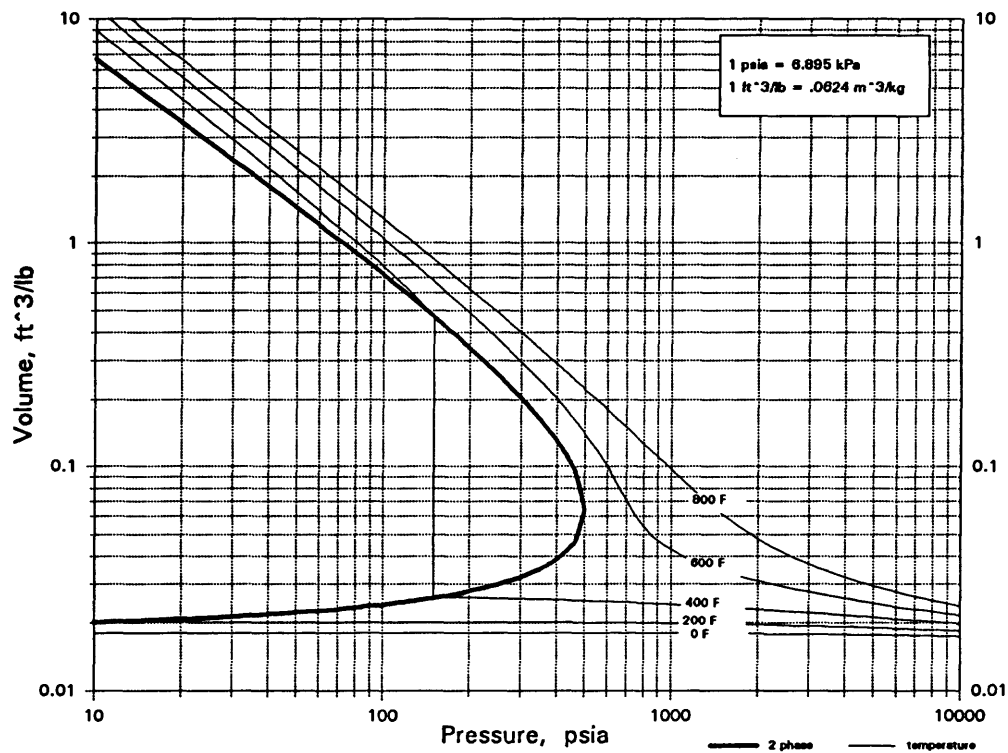
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n-PROPYL ACETATE

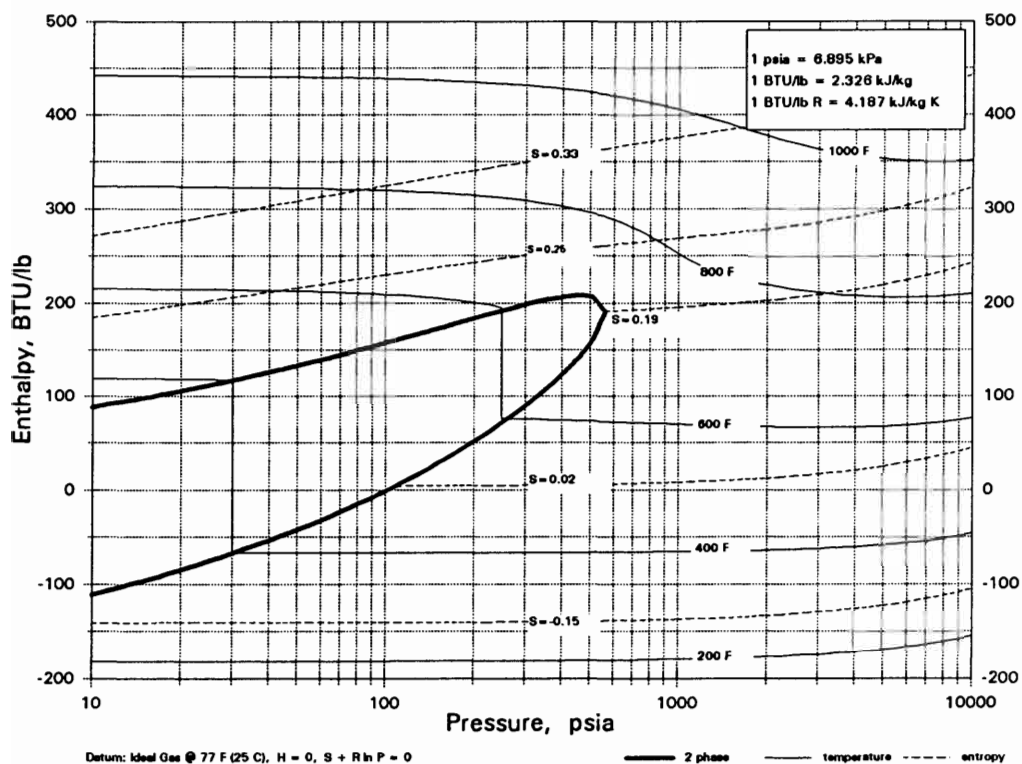
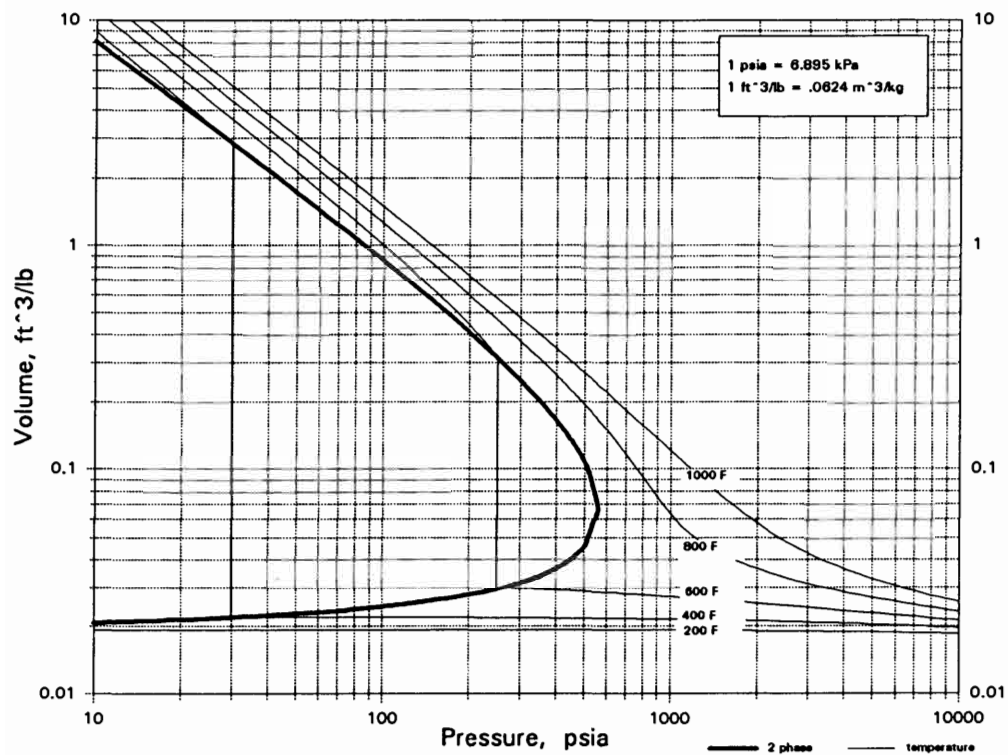


C5H10O2

METHYL n-BUTYRATE

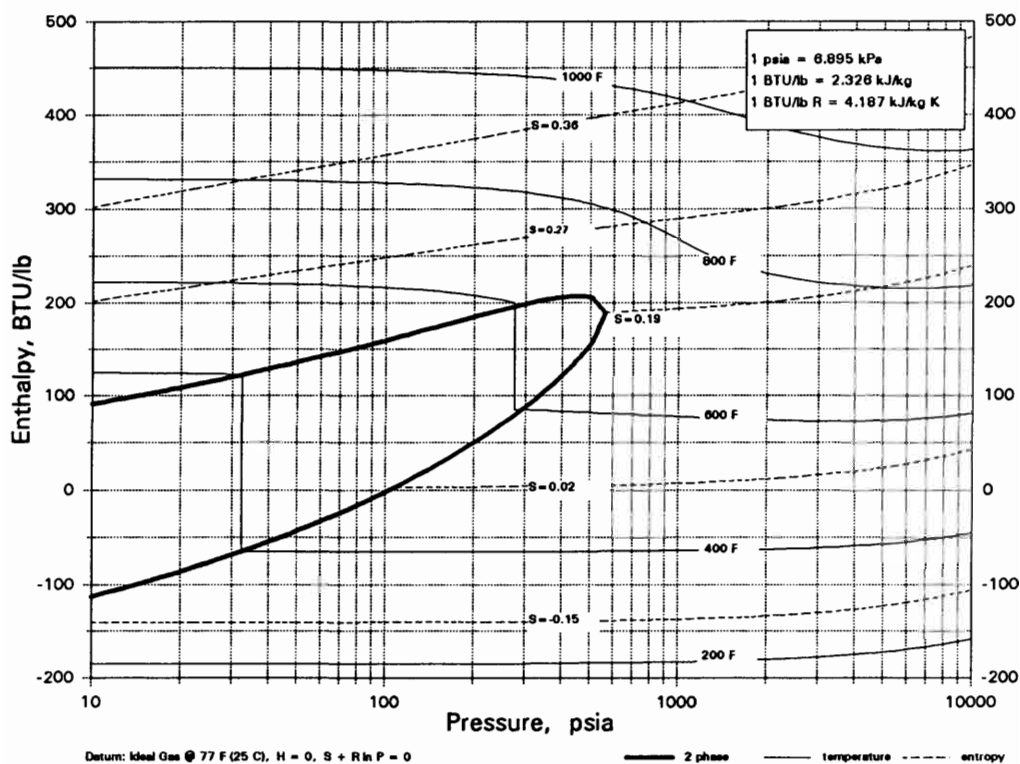
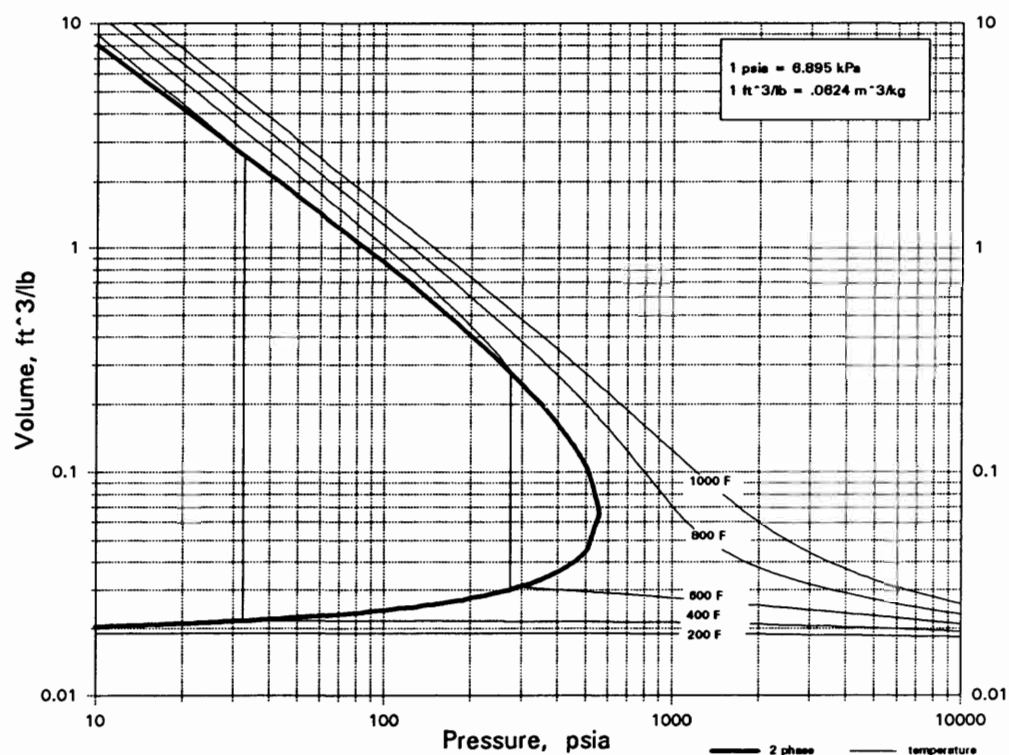


C5H10O2
2-METHYLBUTYRIC ACID



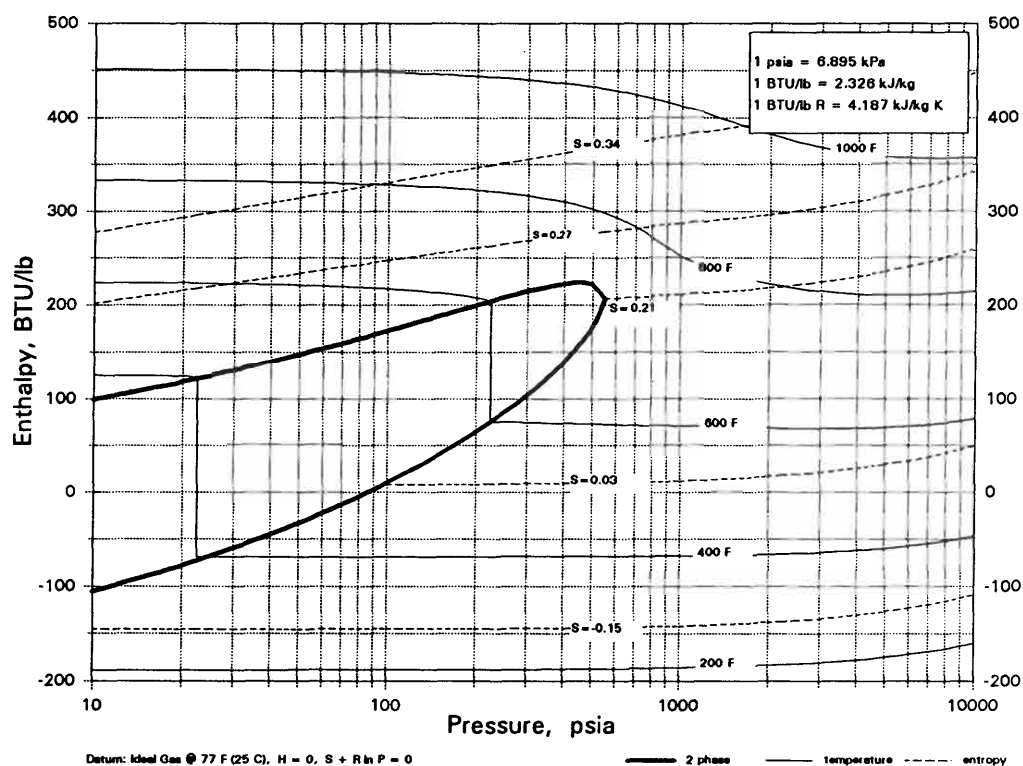
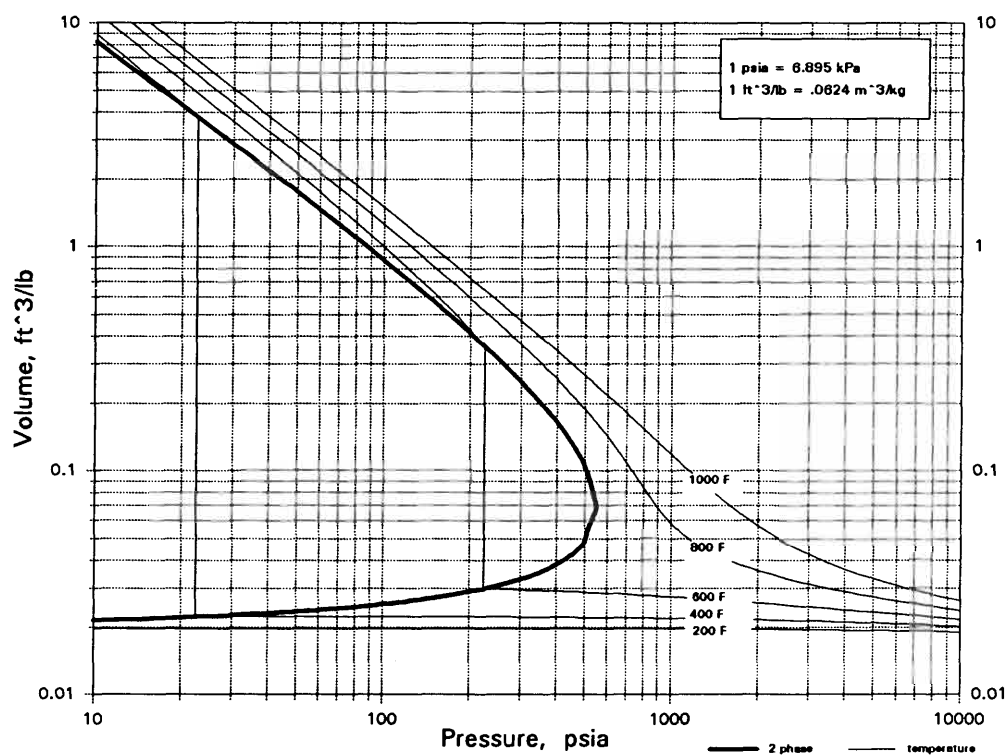
C5H10O2

ISOVALERIC ACID

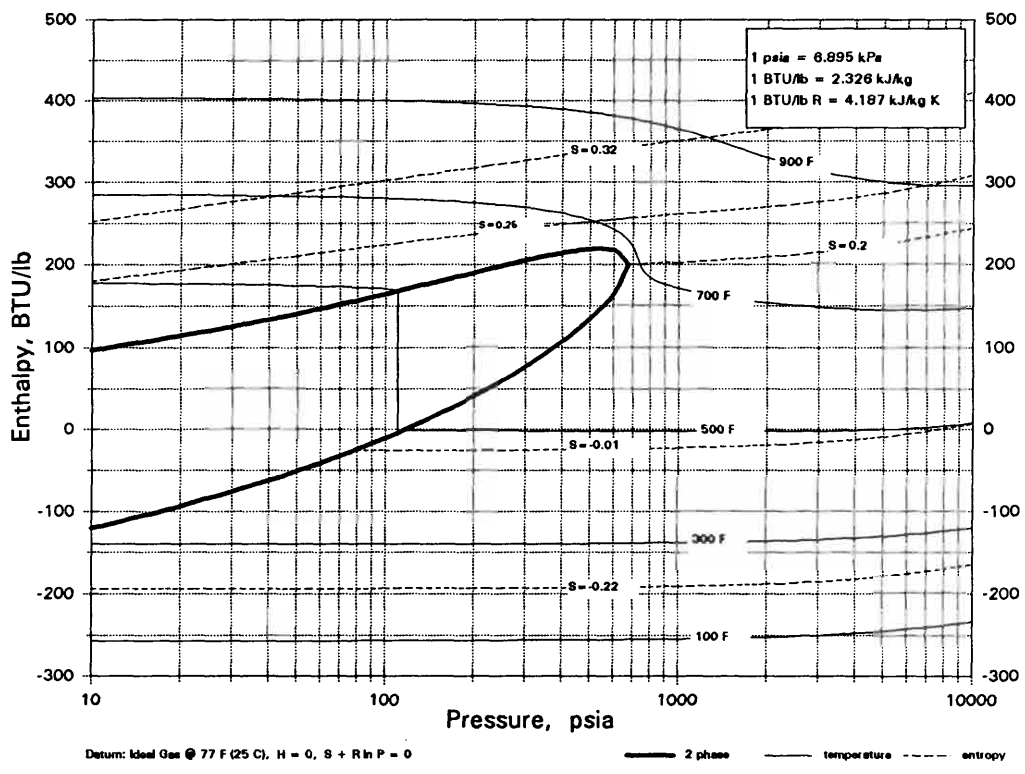
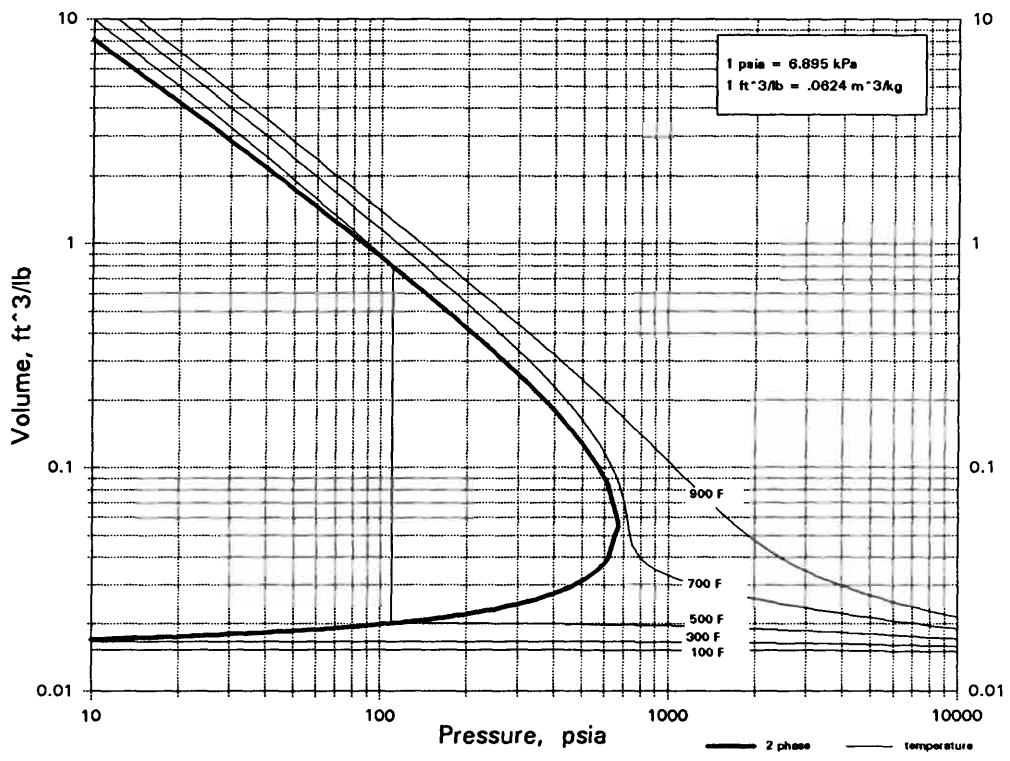


C5H10O2

VALERIC ACID

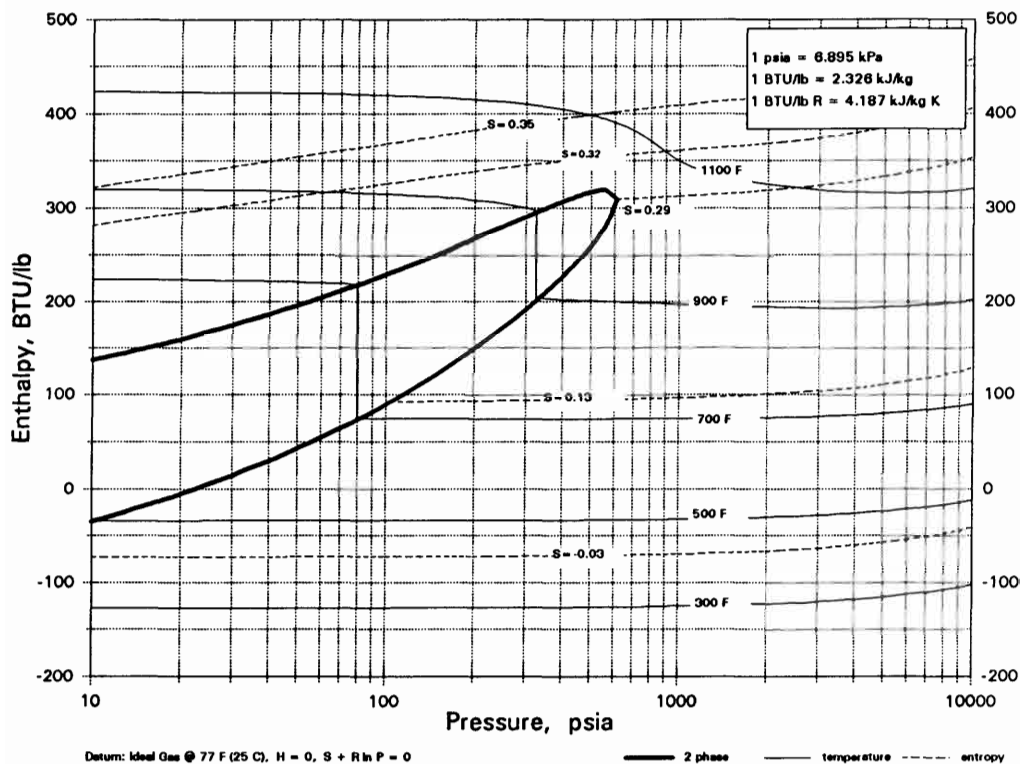
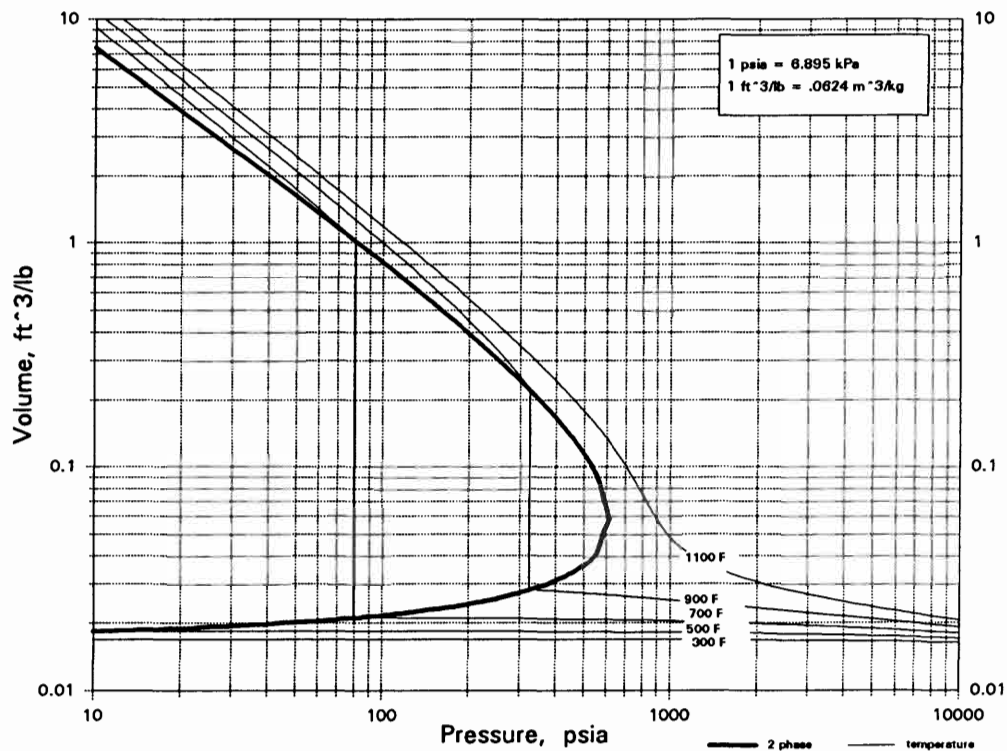


C5H10O2
TETRAHYDROFURFURYL ALCOHOL



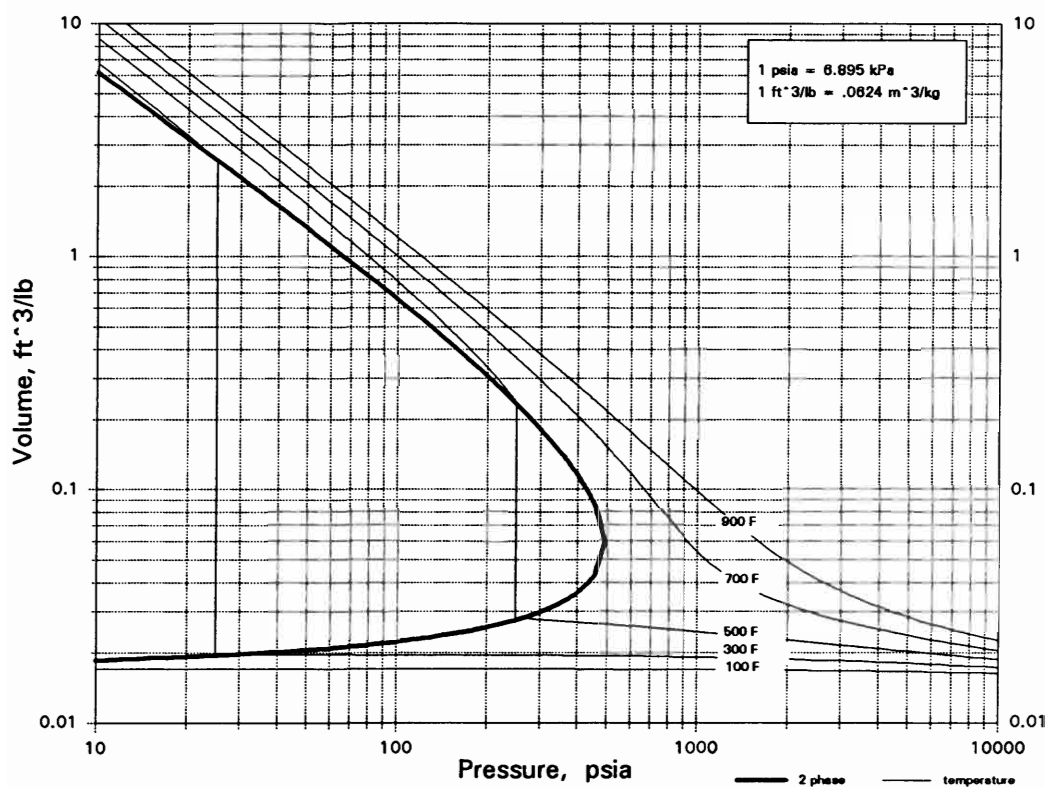
C5H10O2S

3-METHYL SULFOLANE



C5H10O3

DIETHYL CARBONATE



1. Boiling Point, K..... 399.95

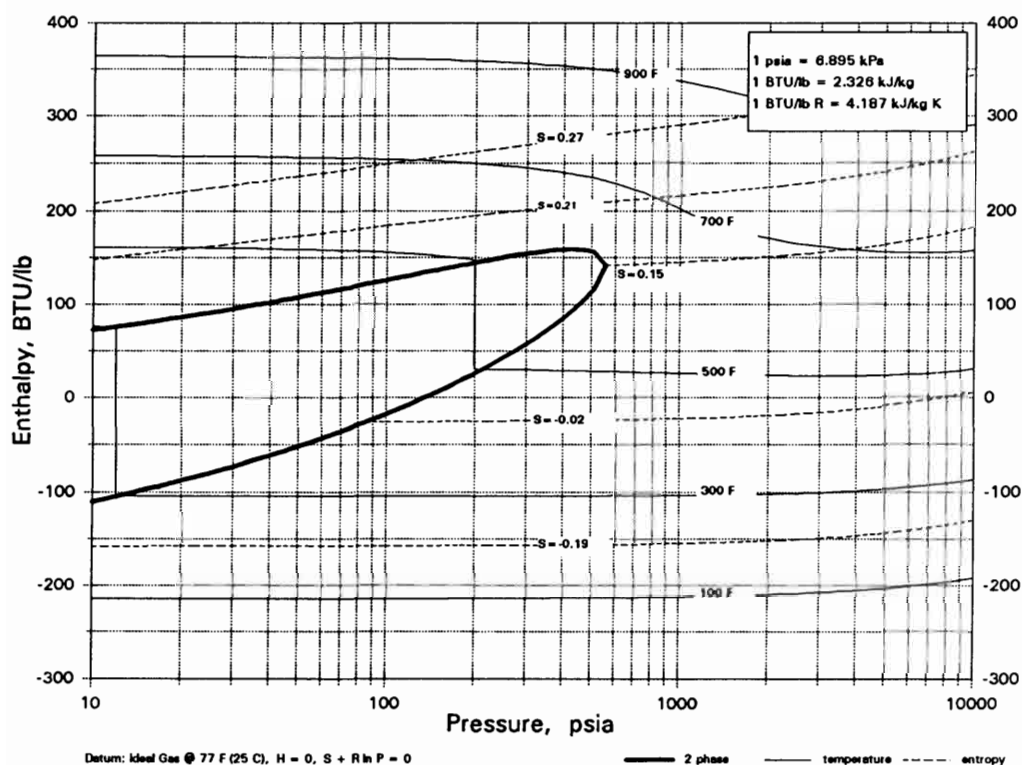
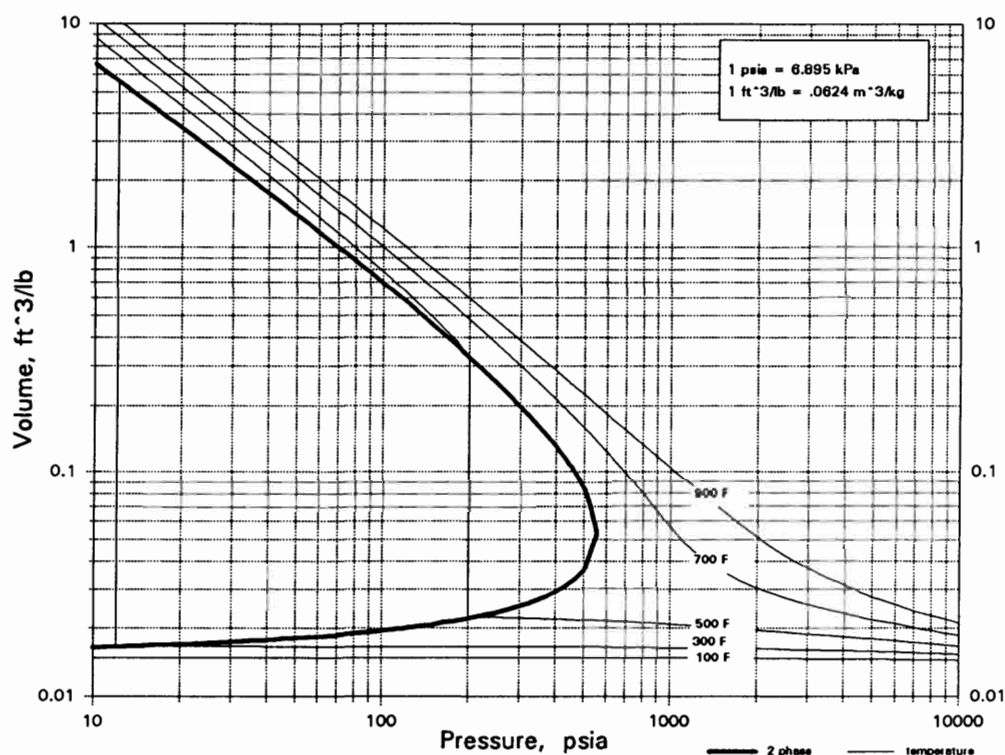
2. Critical Temperature, K.... 576.00

3. Critical Pressure, atm..... 33.46

Heat capacity data are not available.

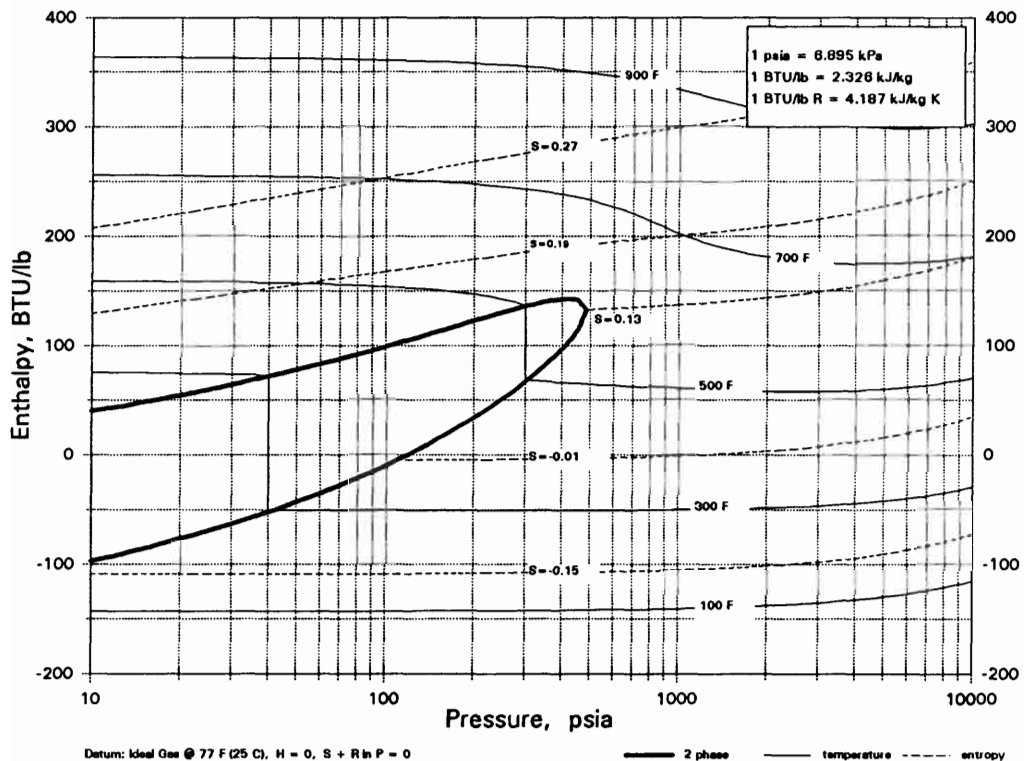
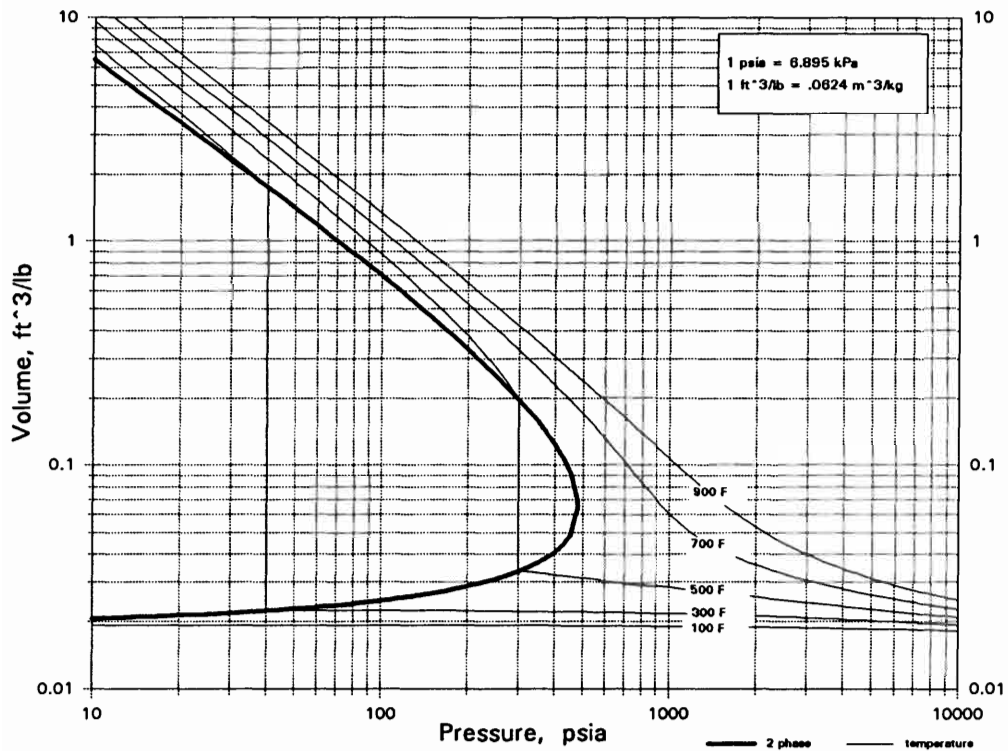
C5H10O3

ETHYL LACTATE



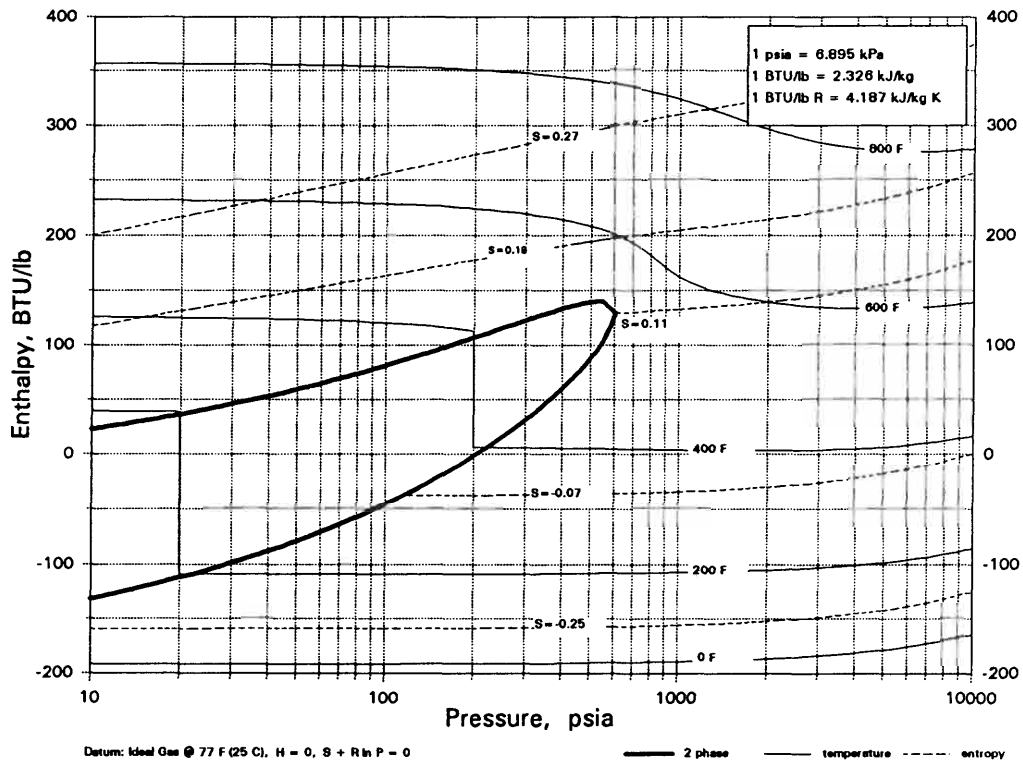
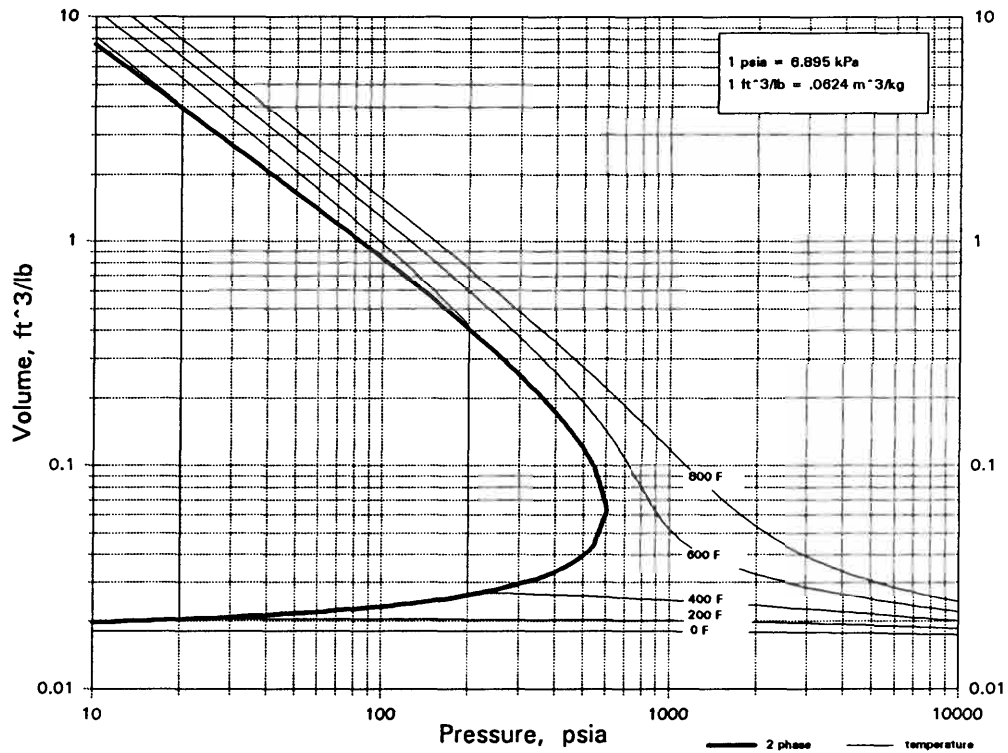
C5H11Cl

1-CHLOROPENTANE



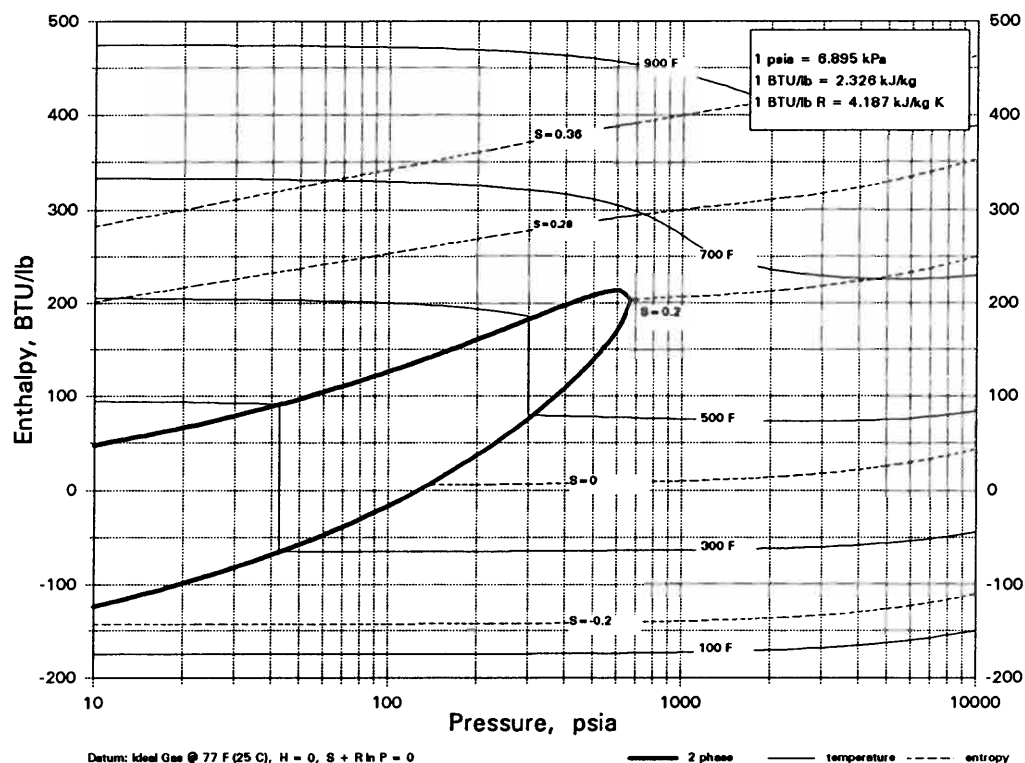
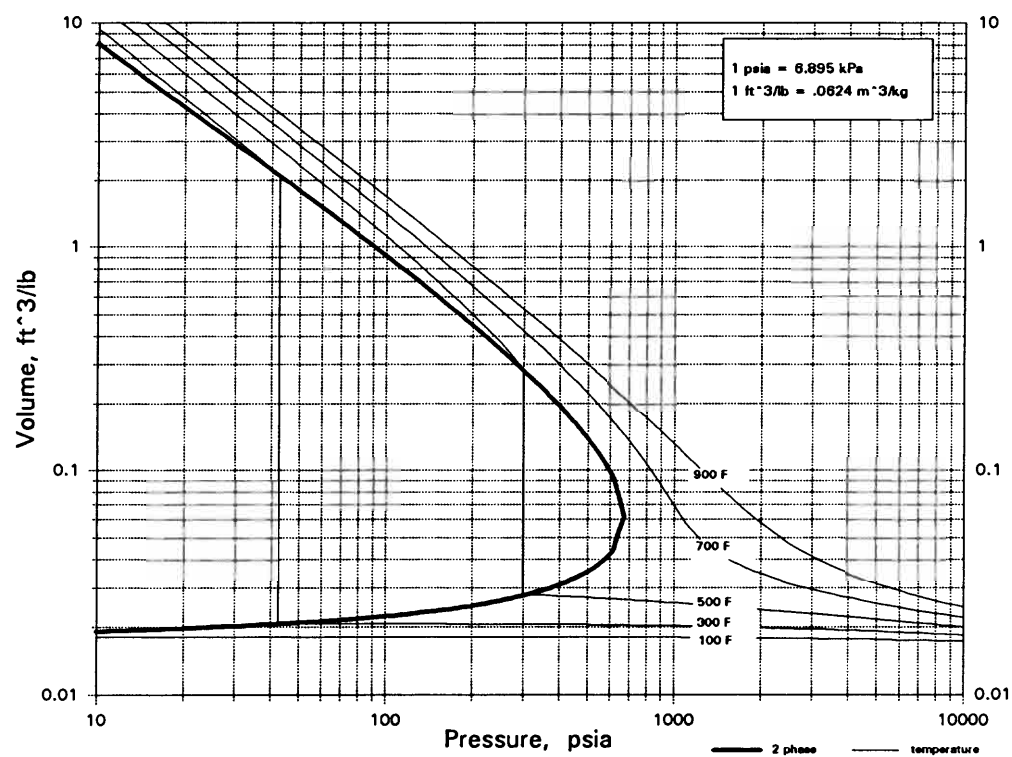
C5H11N

N-METHYLPYRROLIDINE



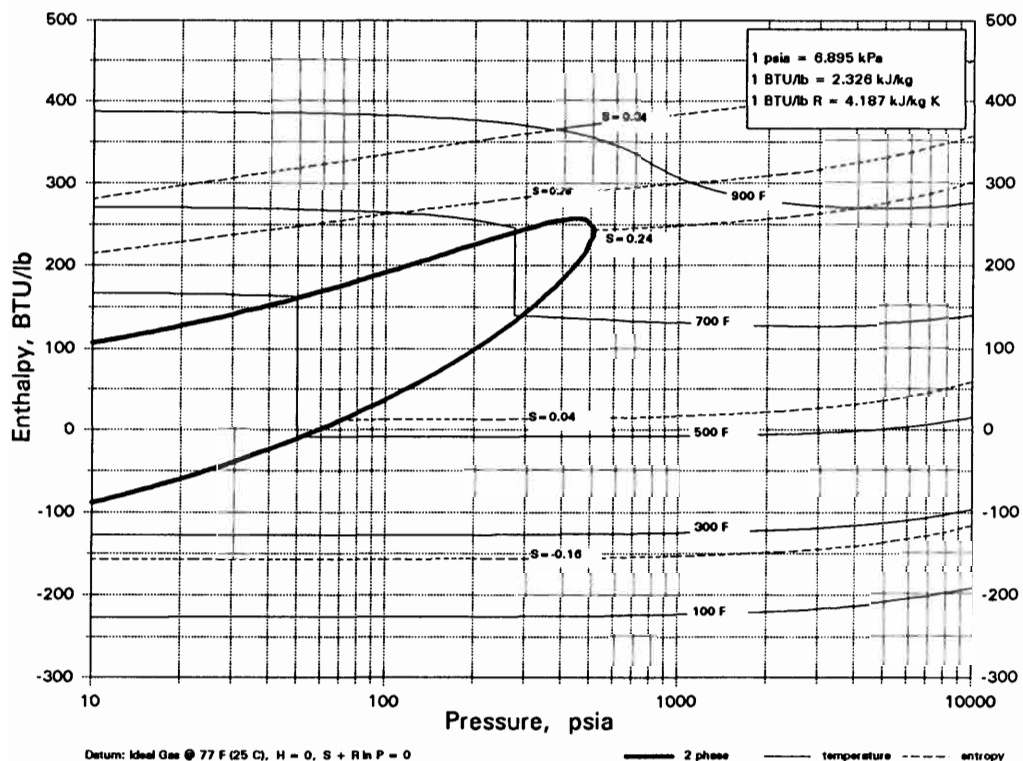
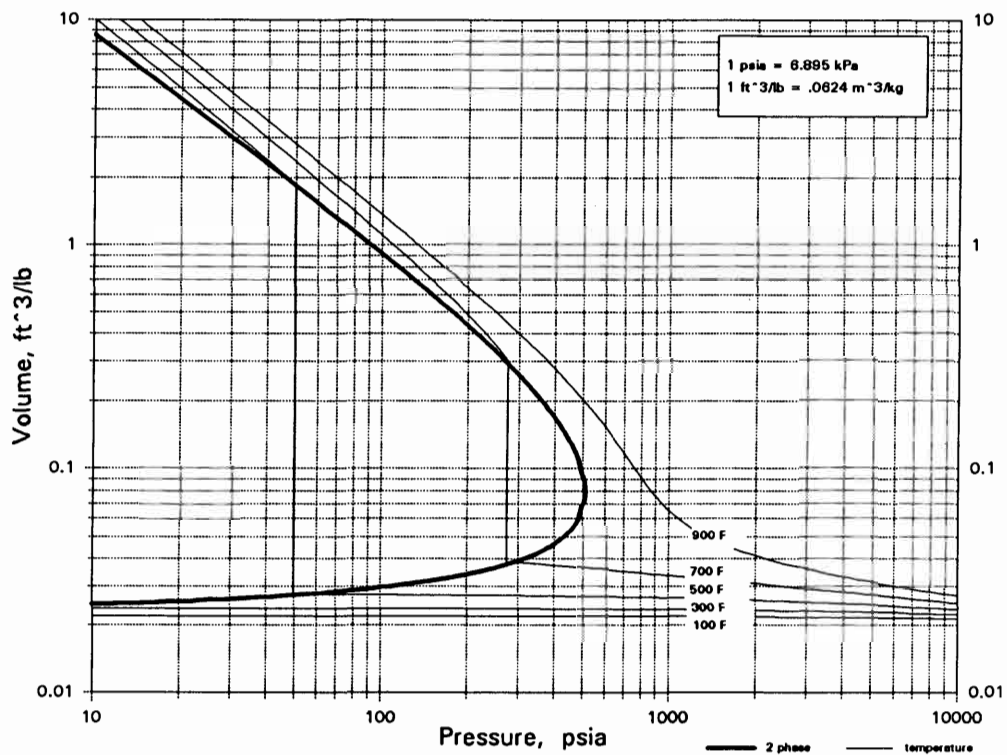
C5H11N

PIPERIDINE



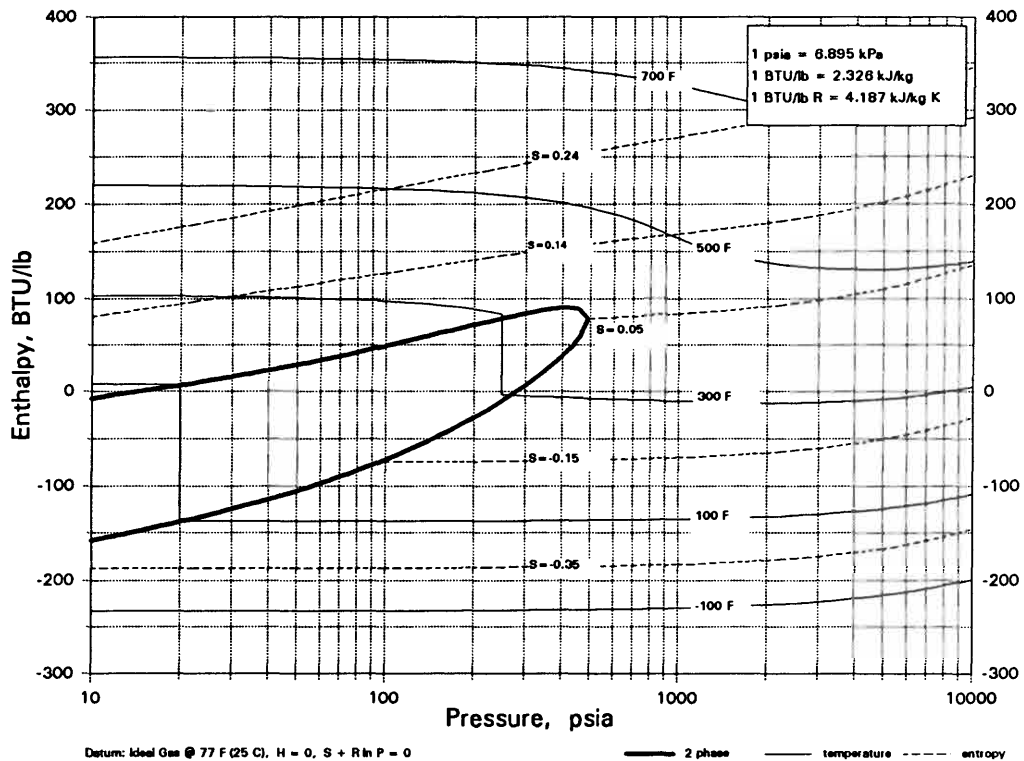
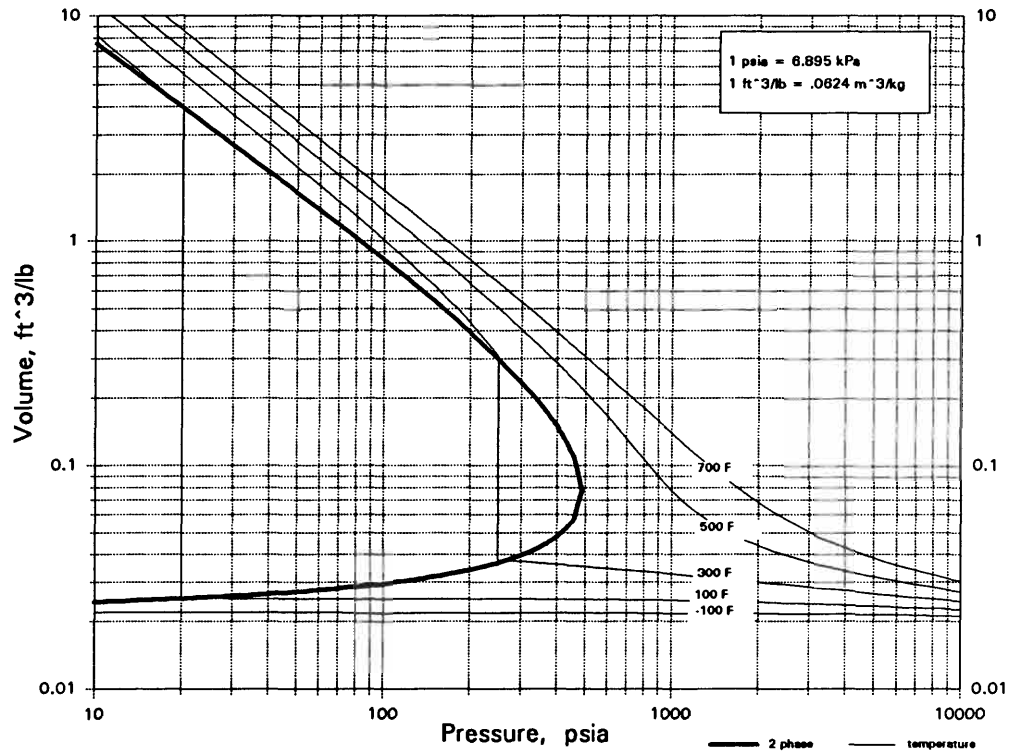
C5H11NO

tert-BUTYLFORMAMIDE



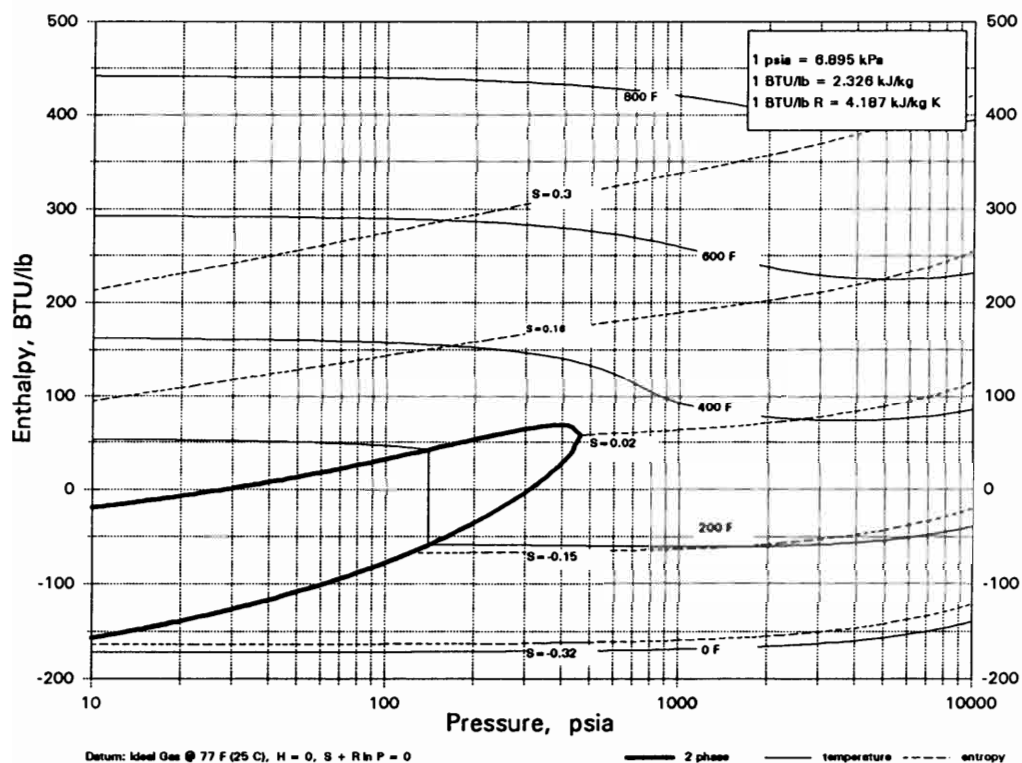
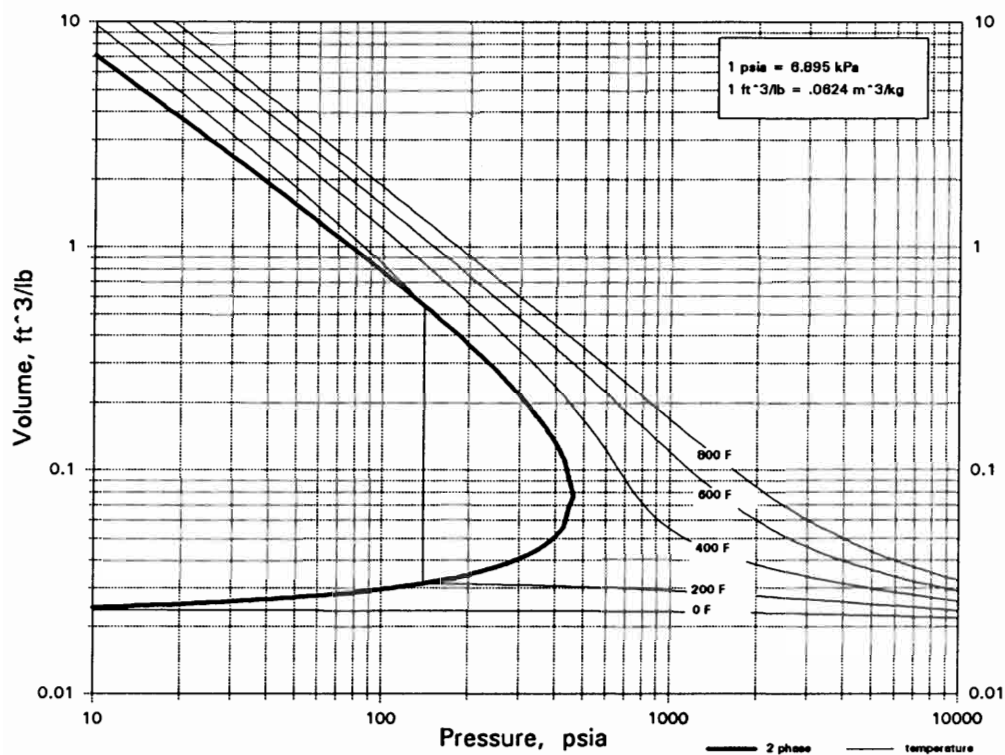
C5H12

ISOPENTANE



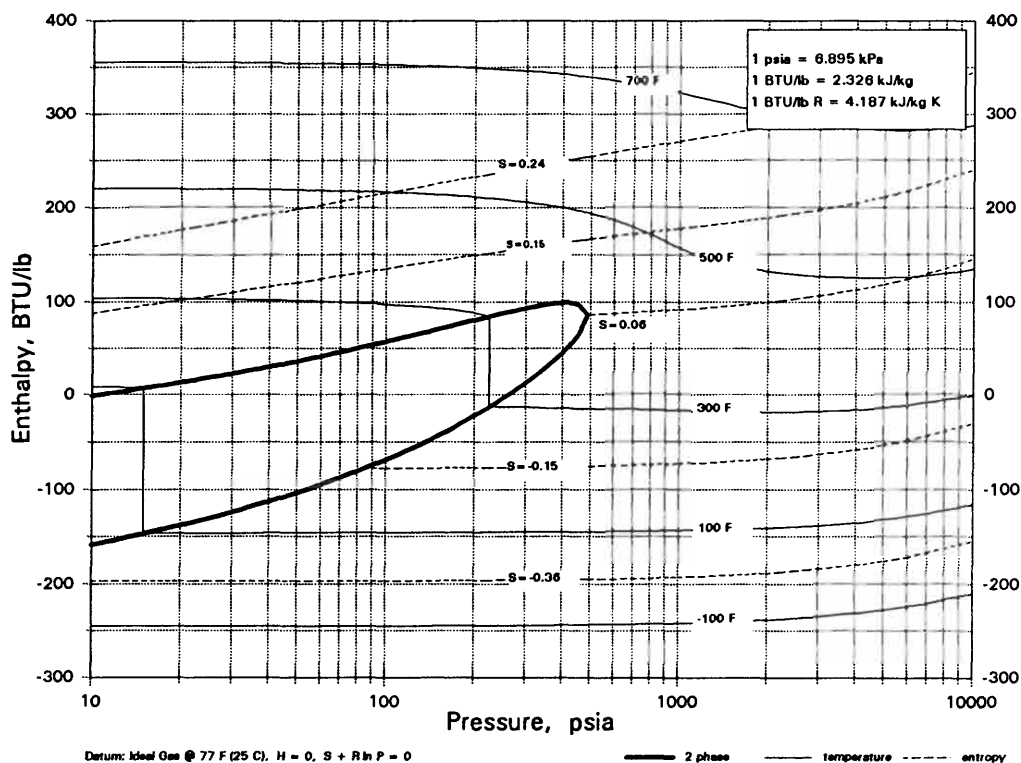
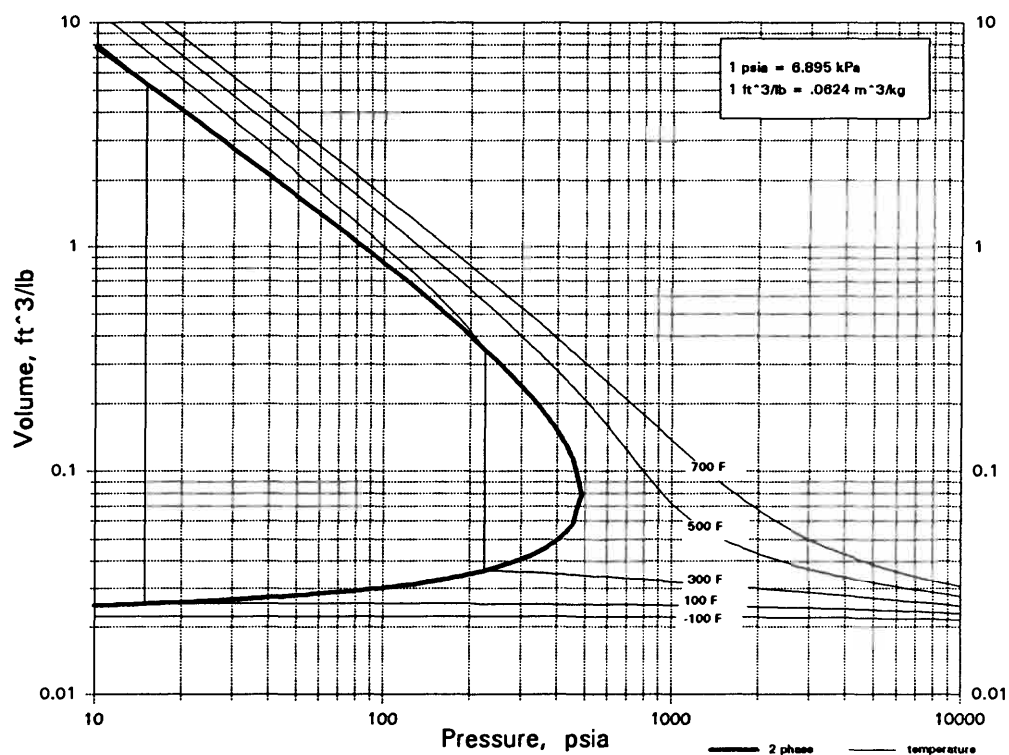
C5H12

NEOPENTANE

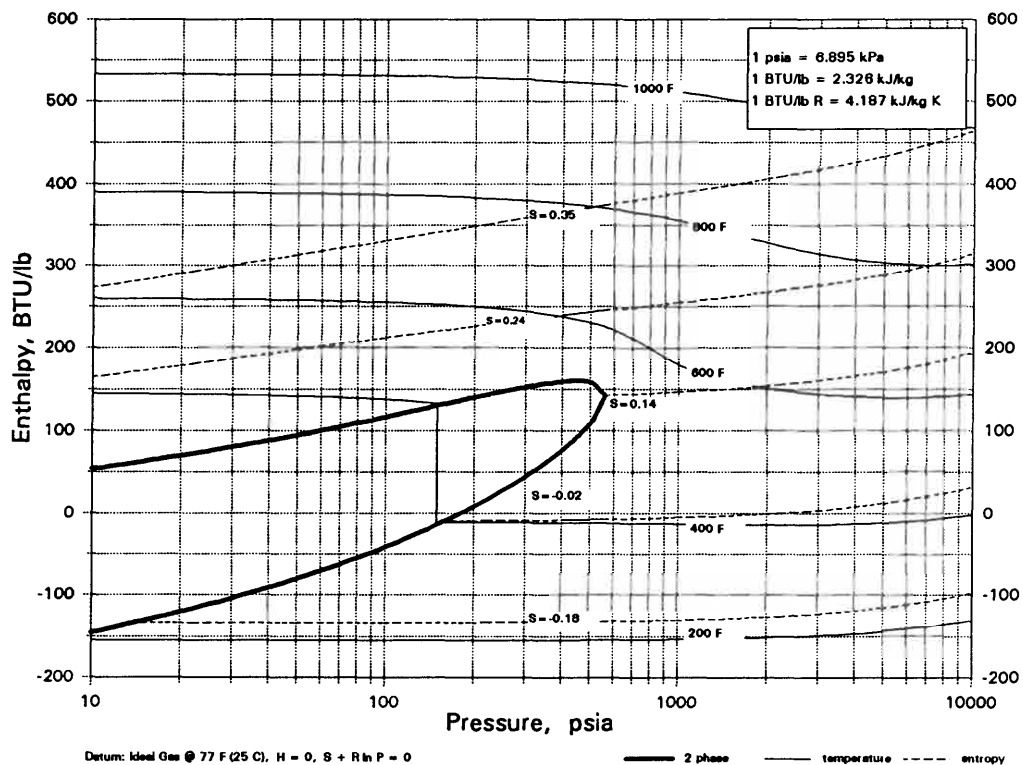
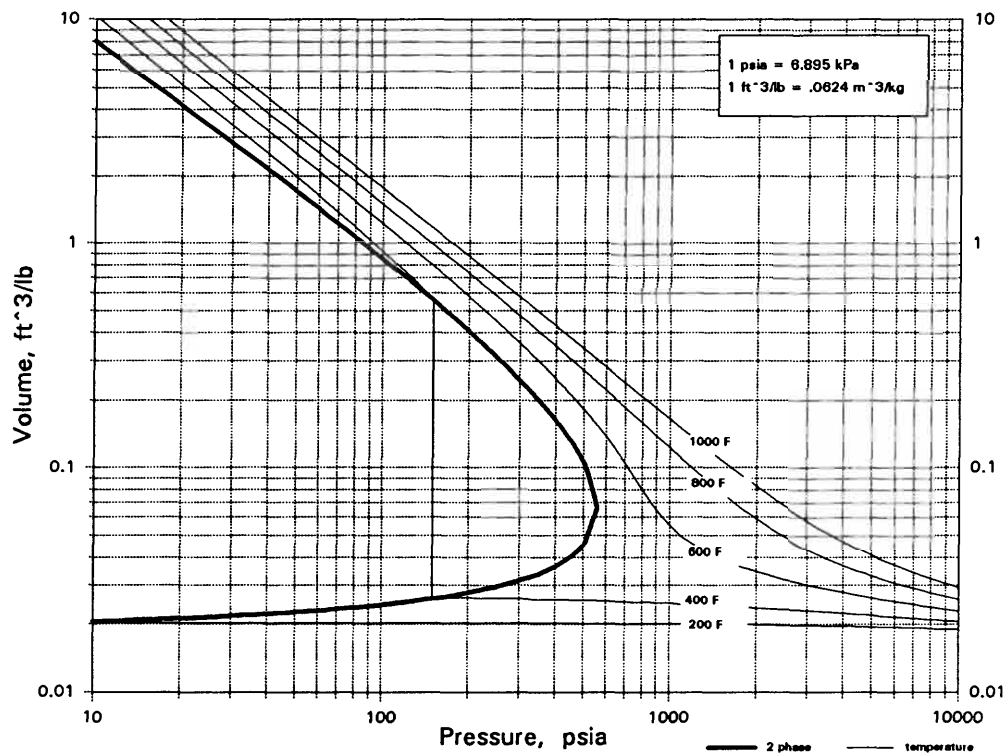


C5H12

n-PENTANE

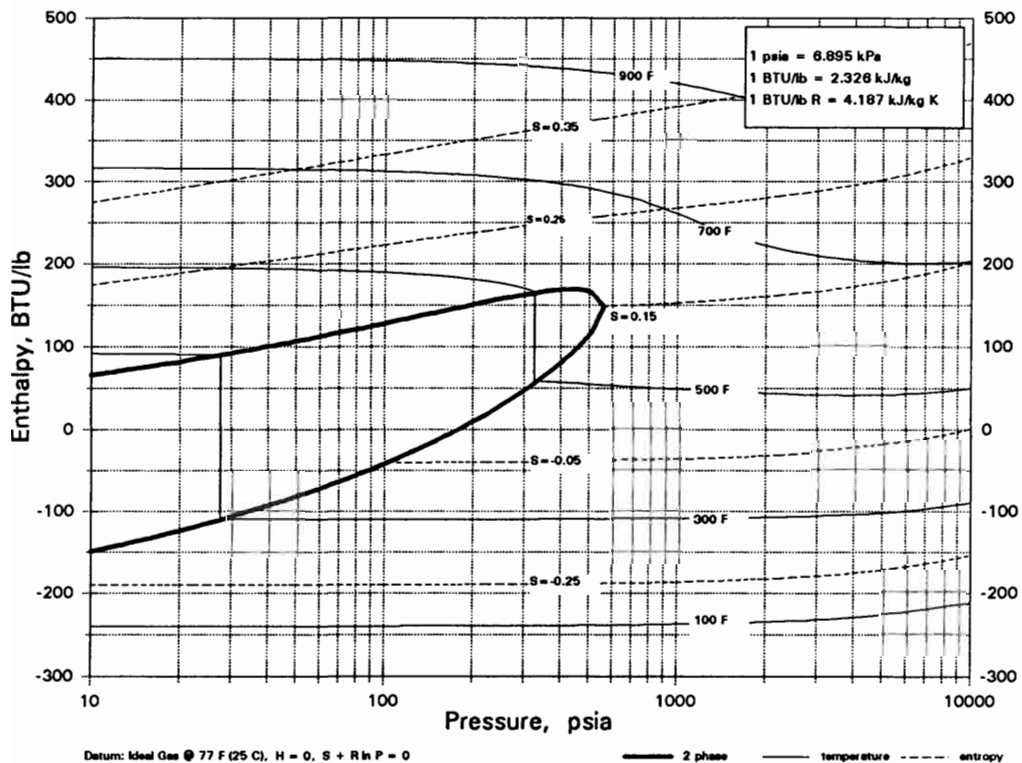
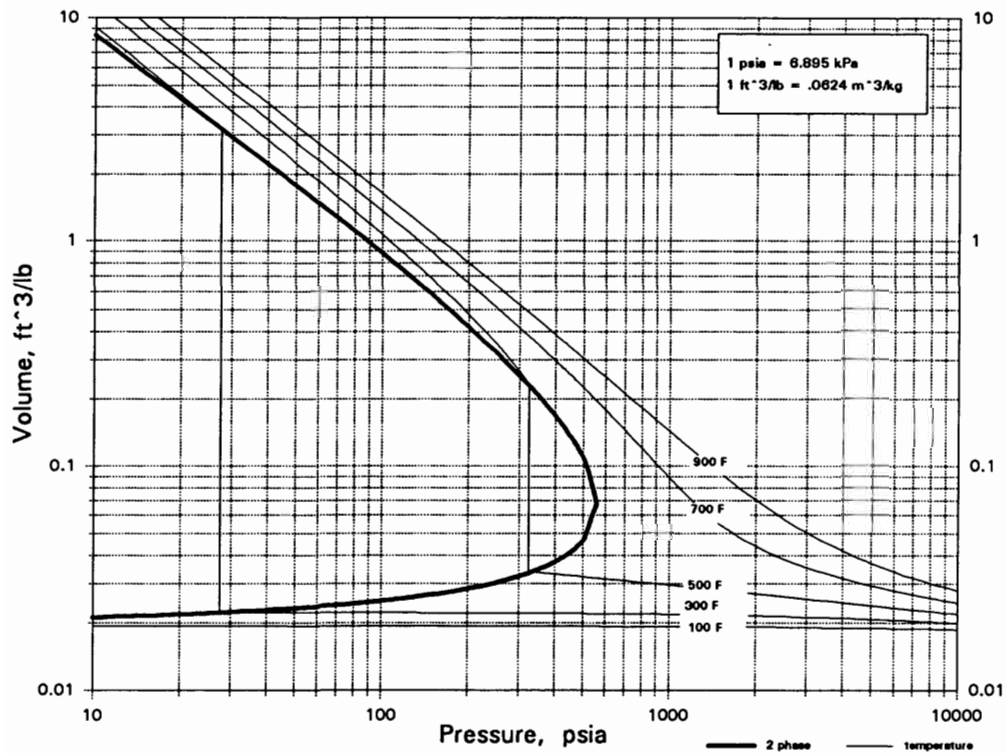


C5H12O
2-2-DIMETHYL-1-PROPANOL



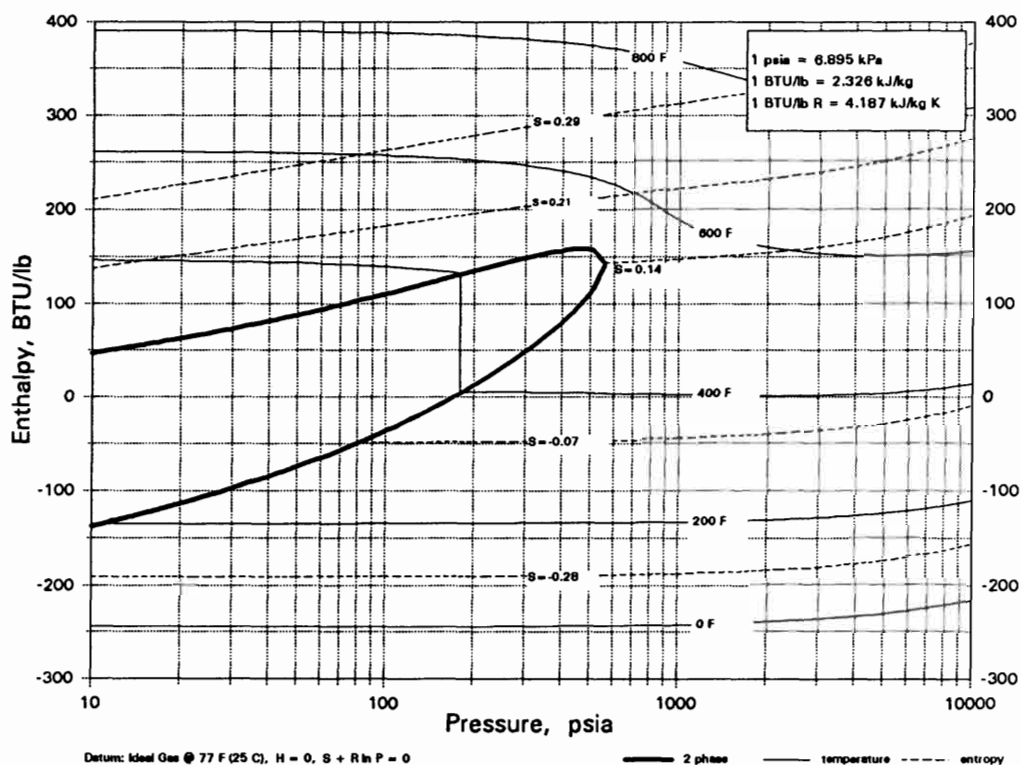
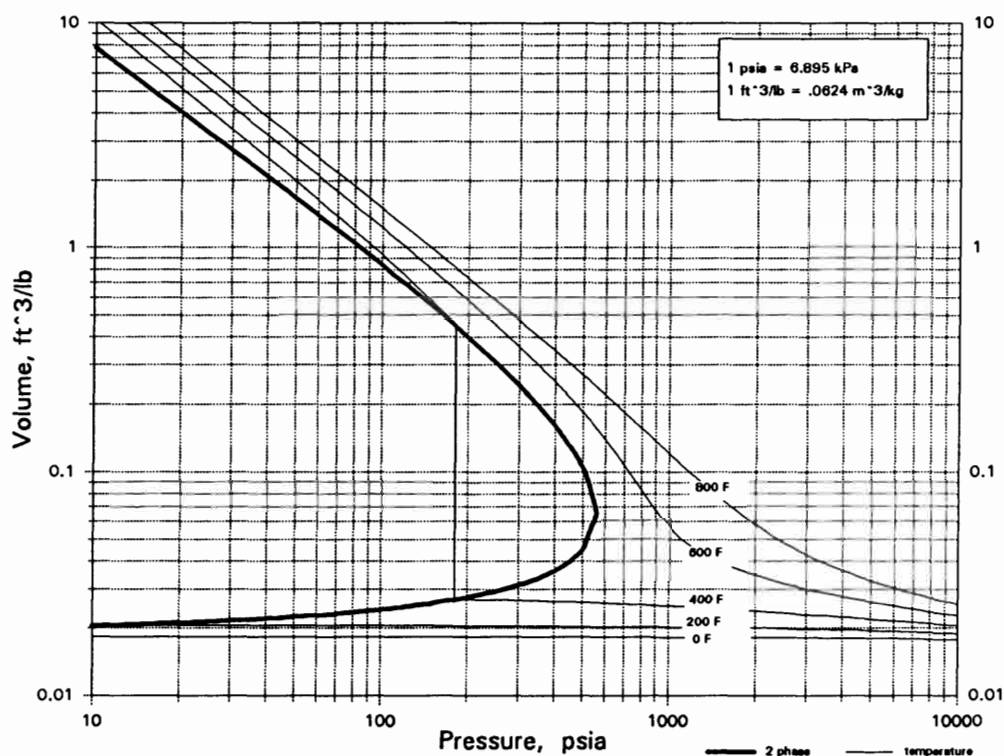
C5H12O

2-METHYL-1-BUTANOL



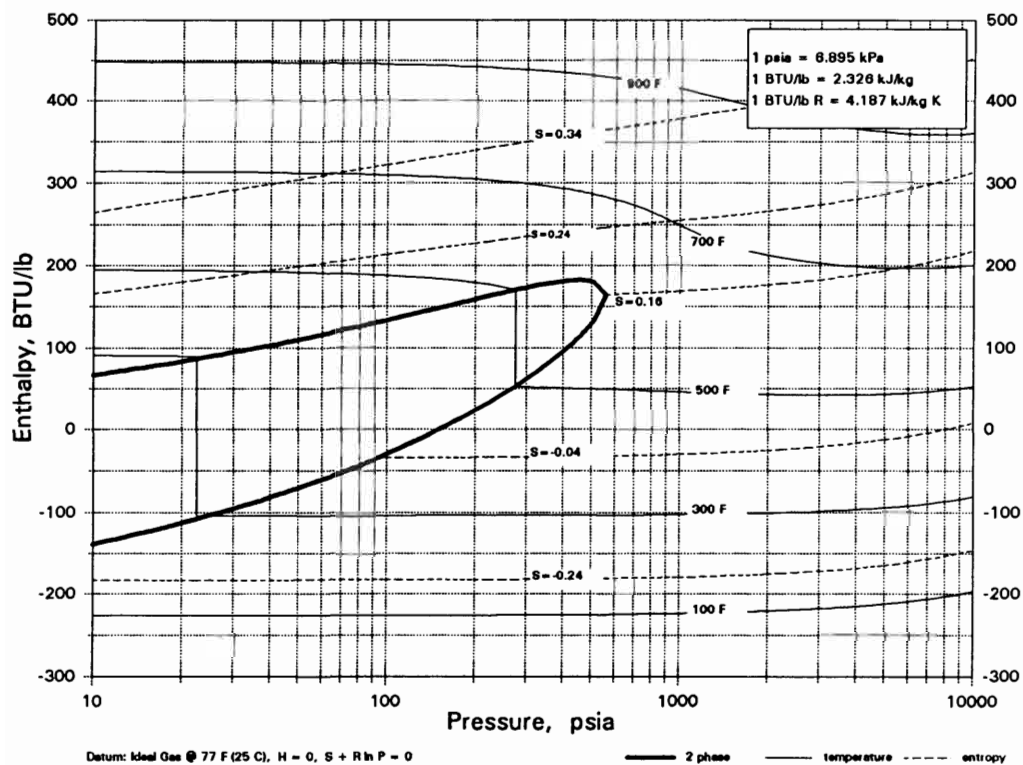
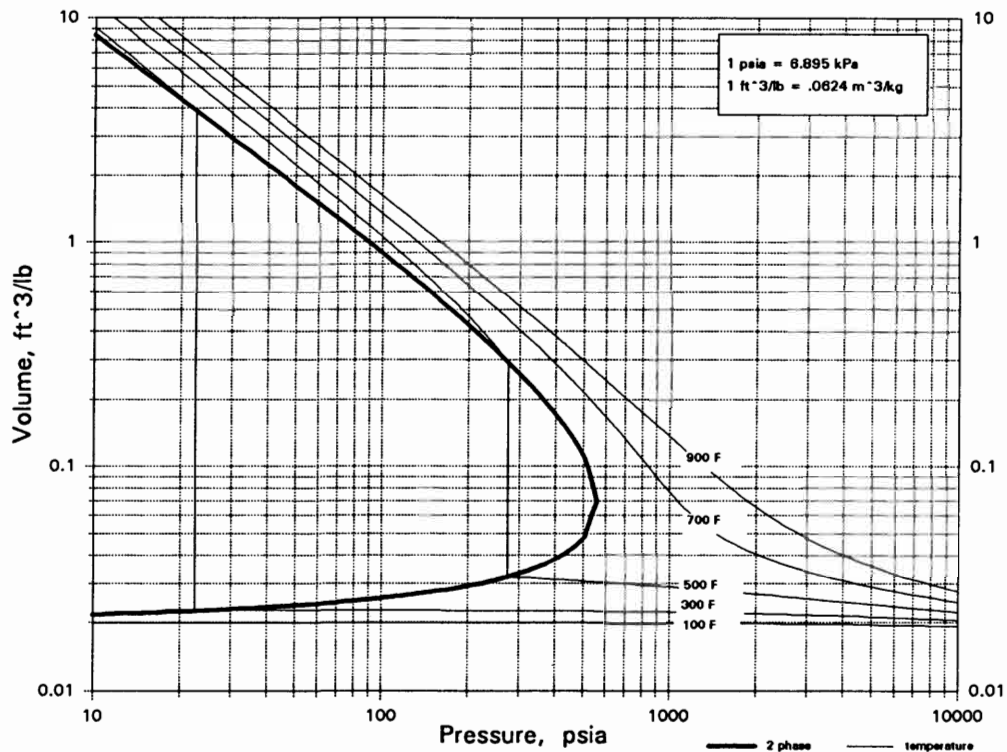
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2-METHYL-2-BUTANOL



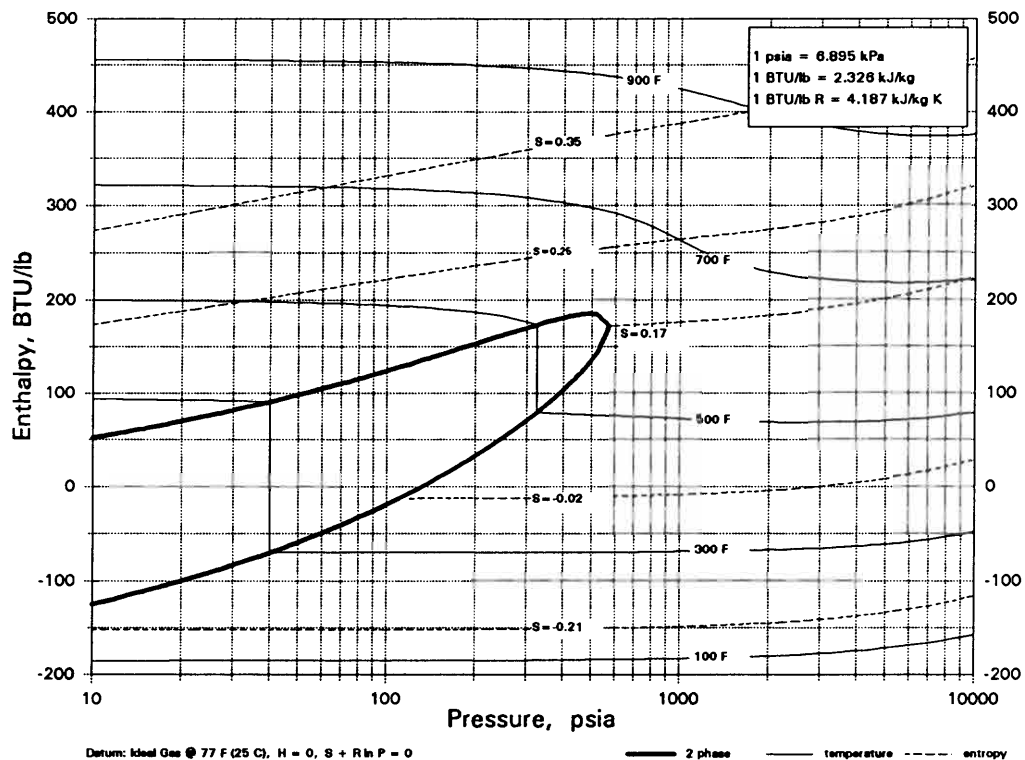
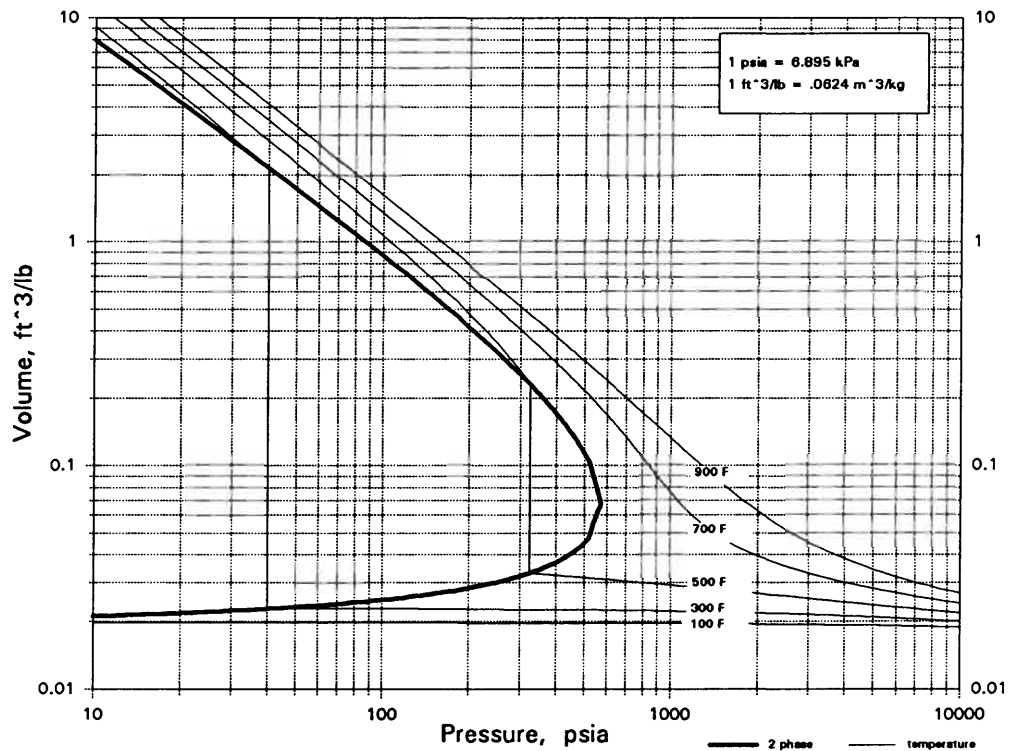
C5H12O

3-METHYL-1-BUTANOL



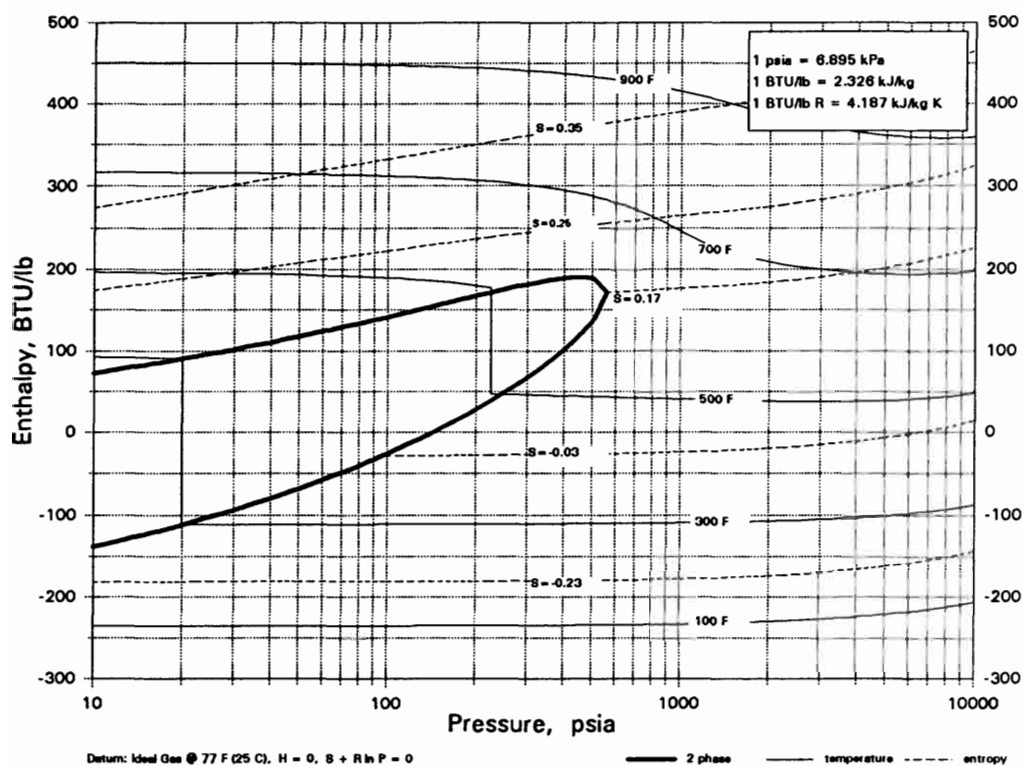
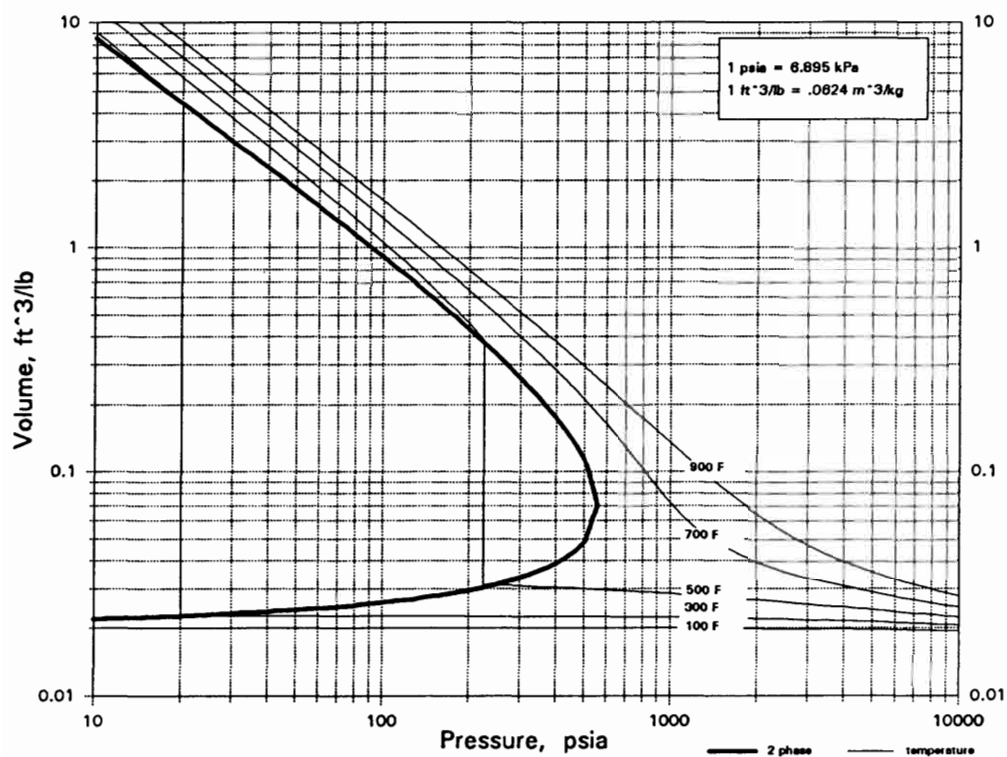
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3-METHYL-2-BUTANOL

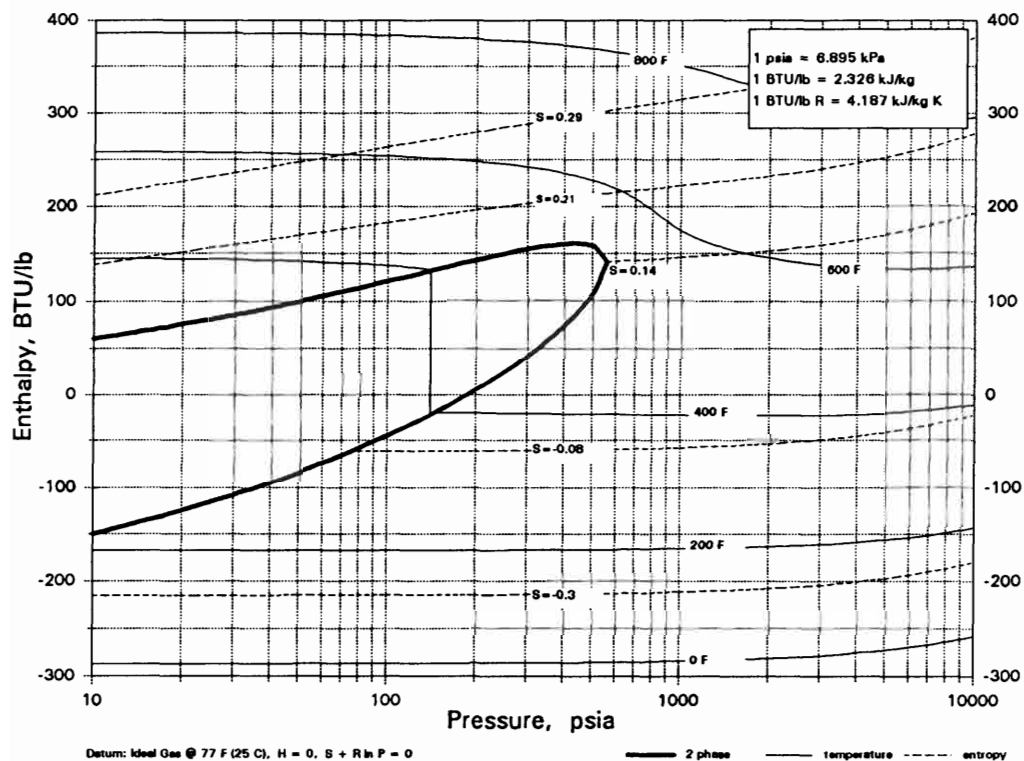
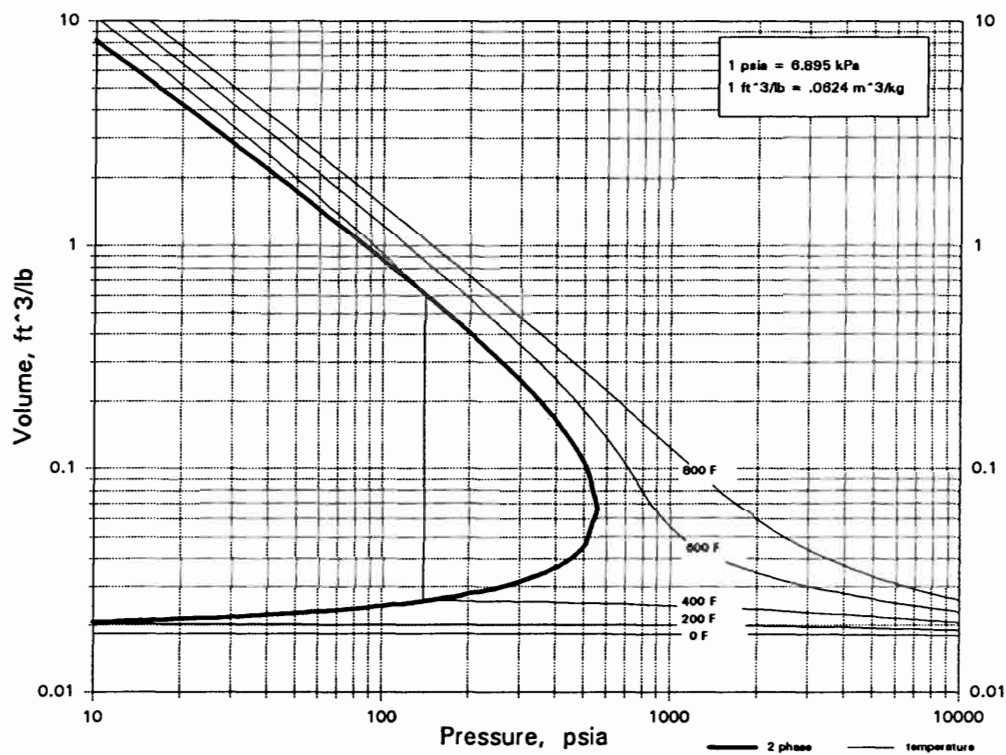


C5H12O

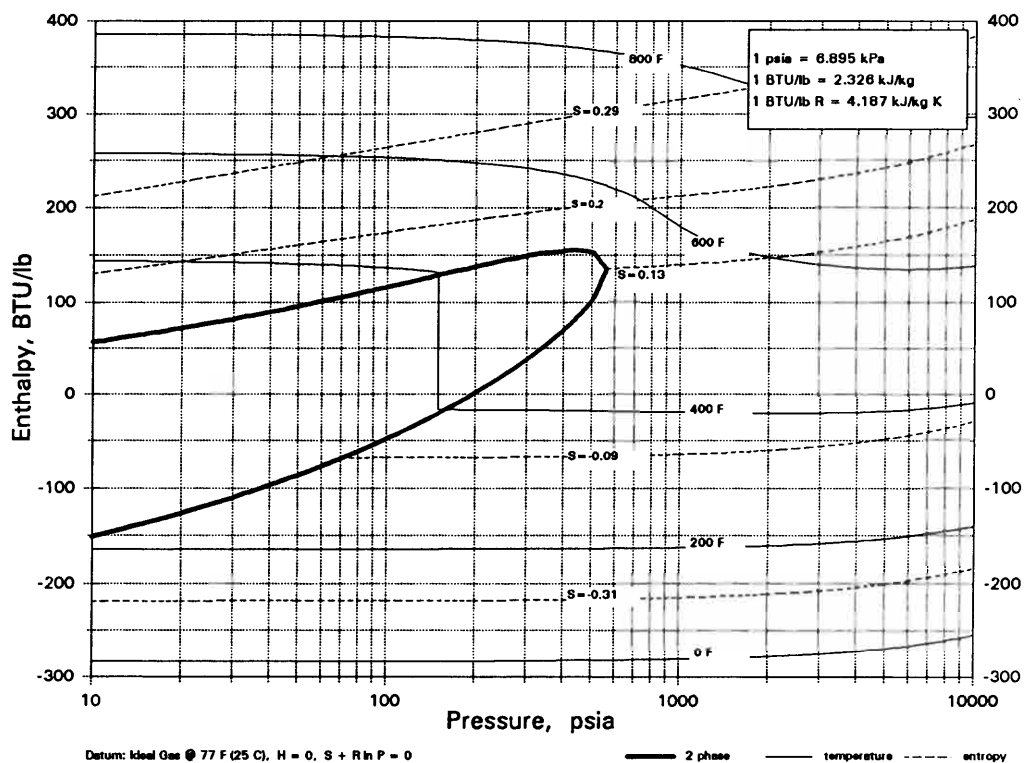
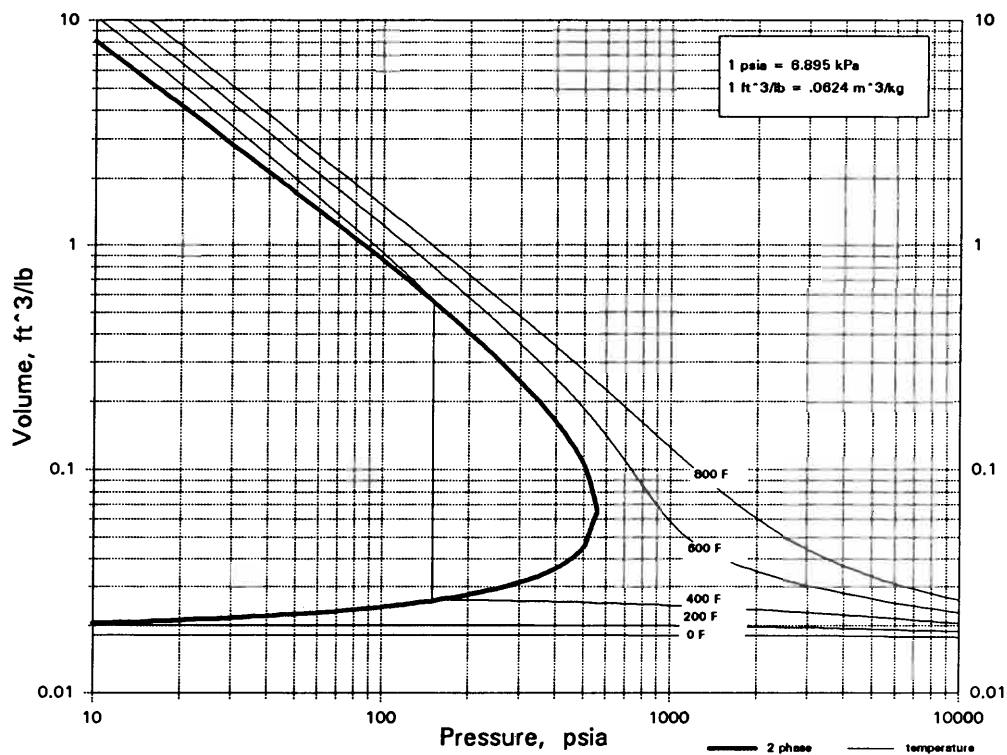
1-PENTANOL



C5H12O
2-PENTANOL

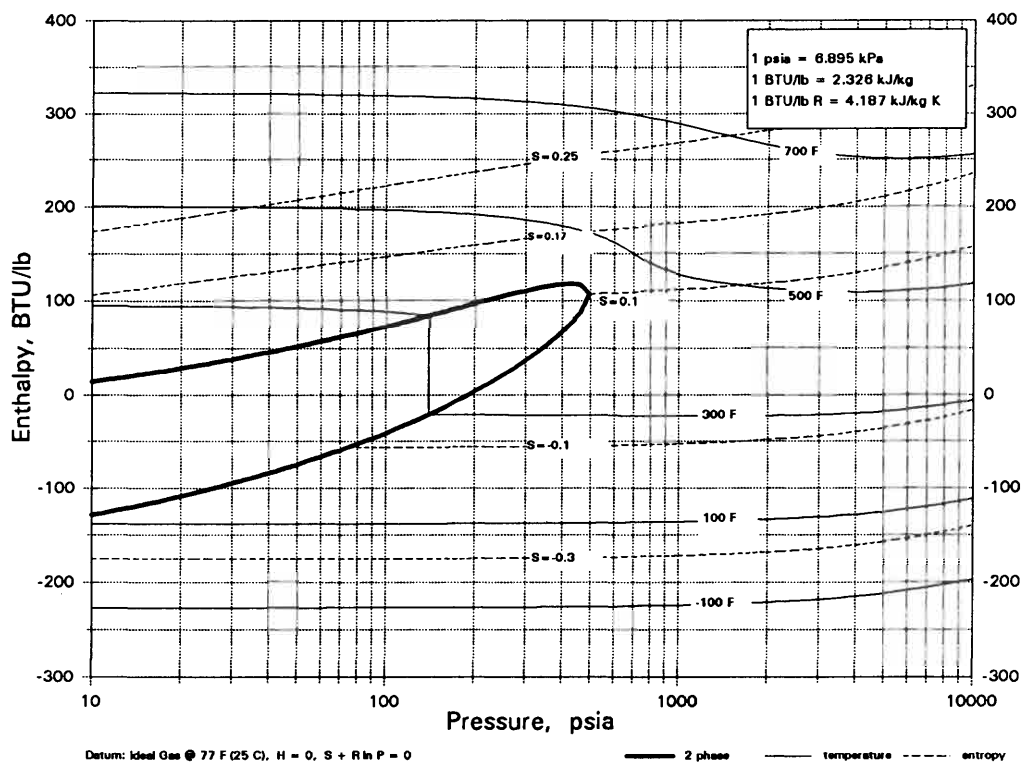
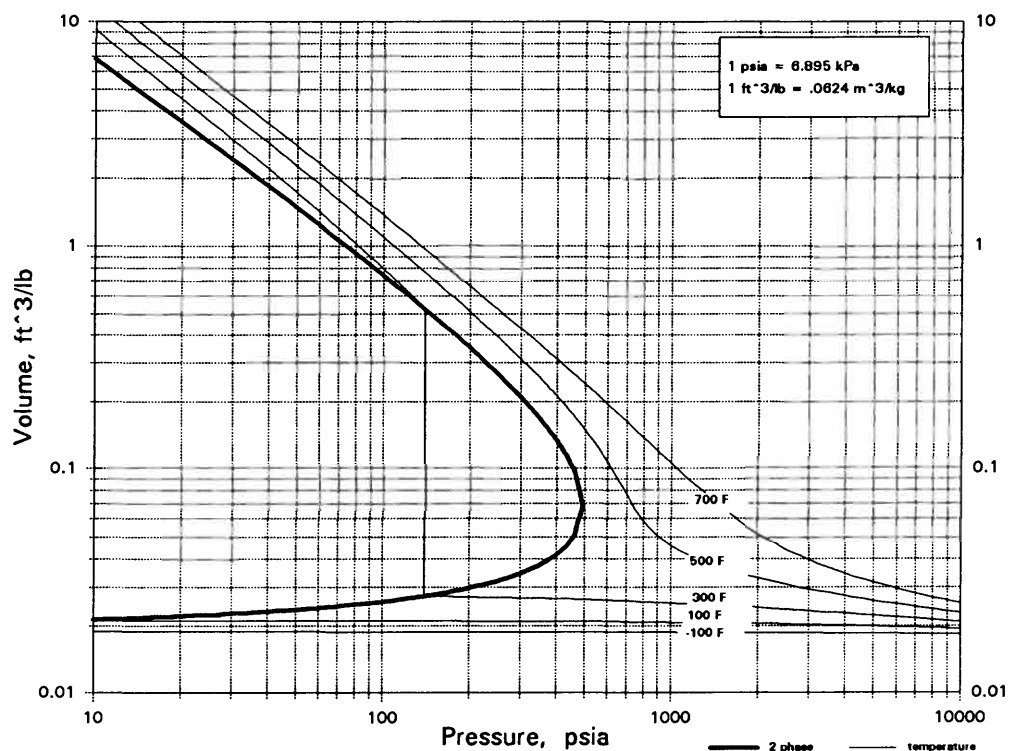


C5H12O
3-PENTANOL



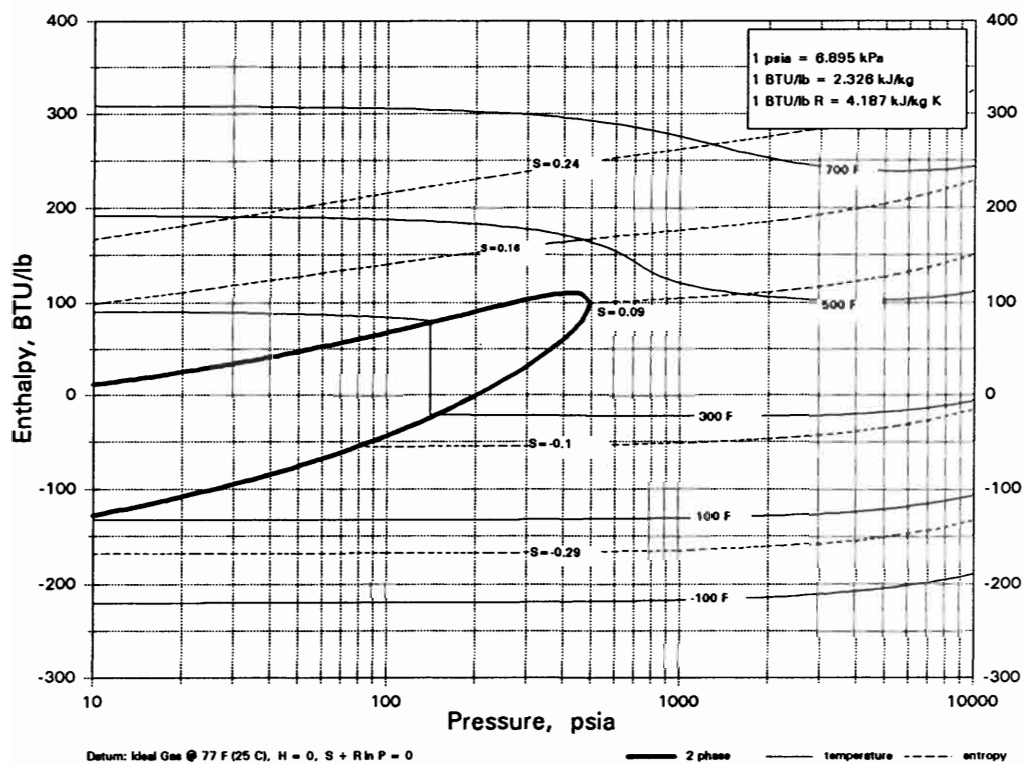
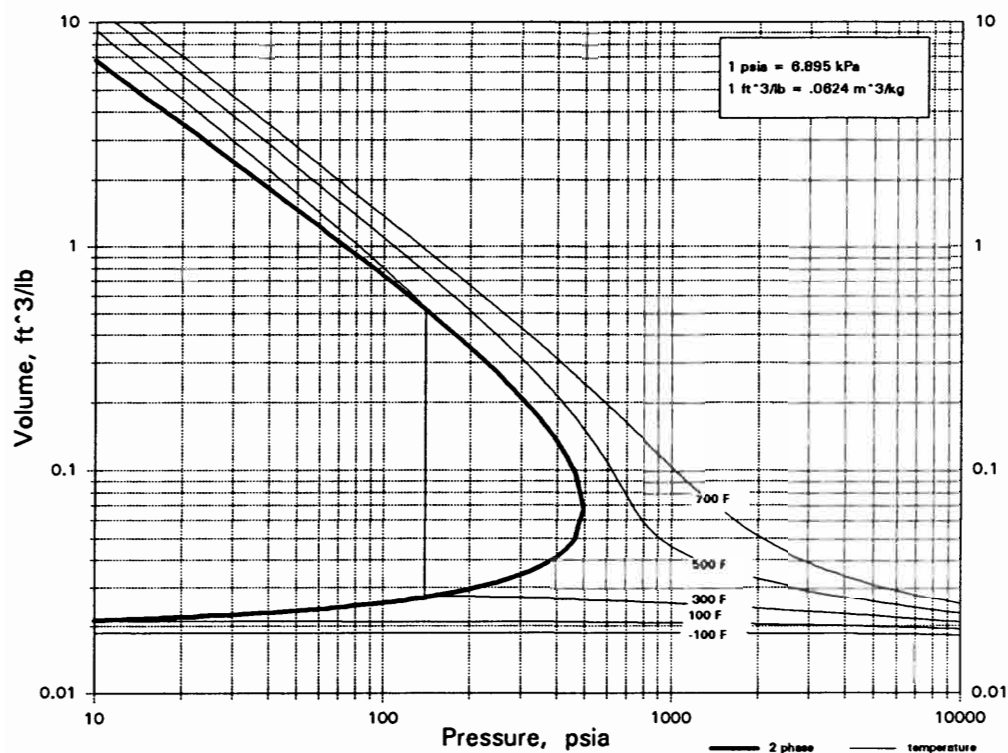
C5H12O

METHYL sec-BUTYL ETHER



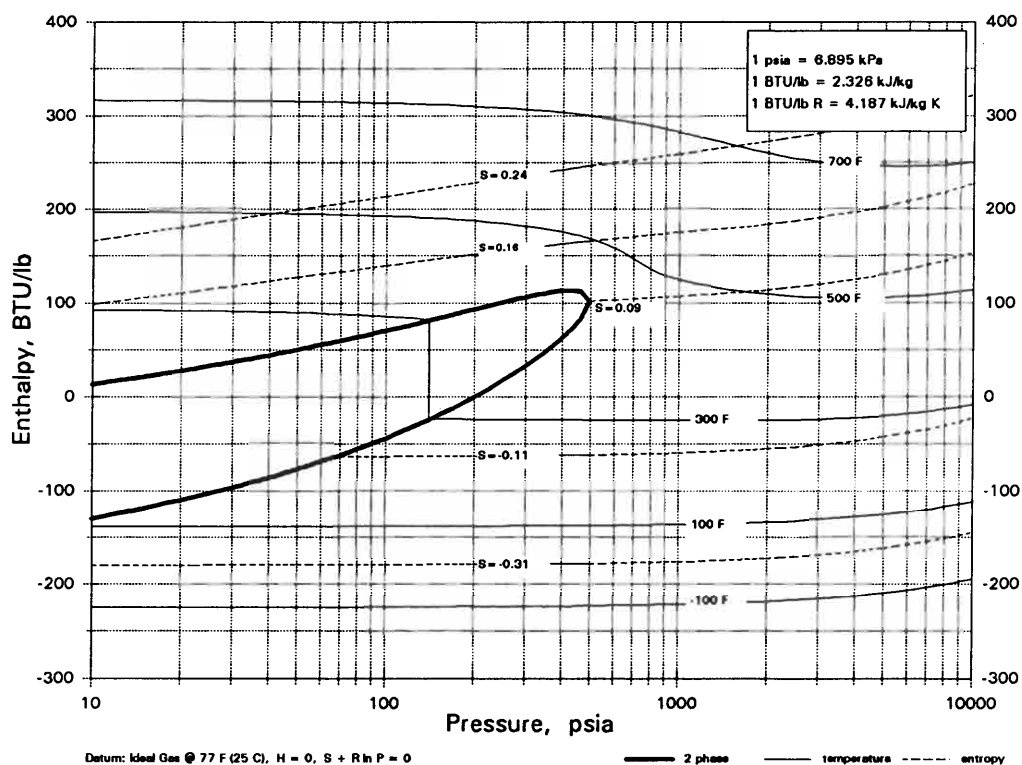
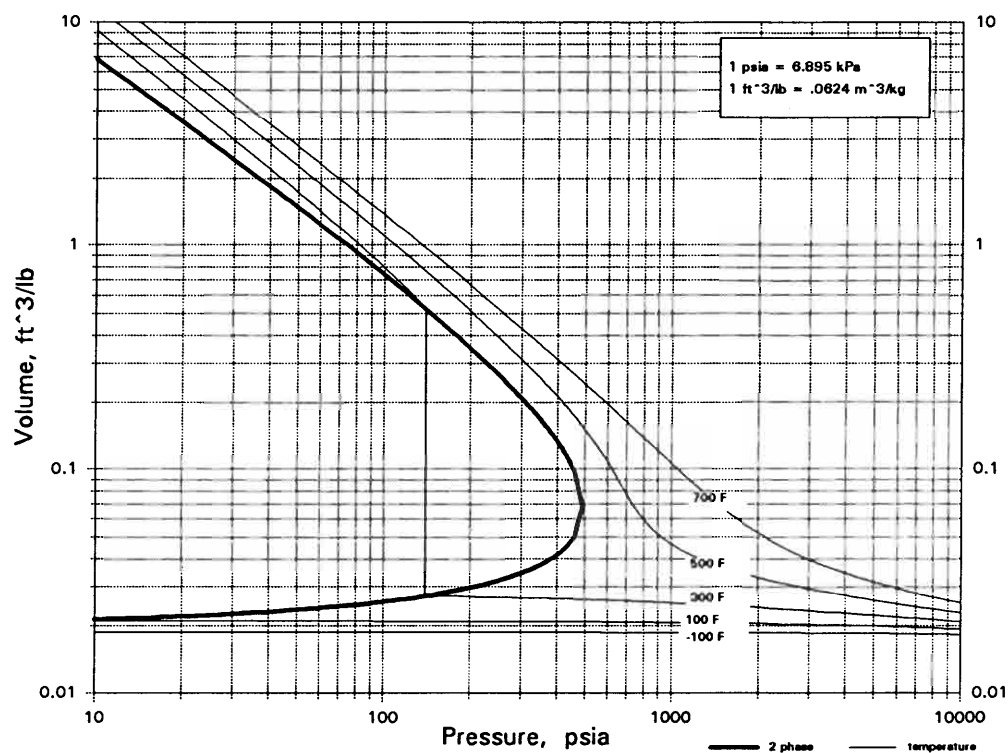
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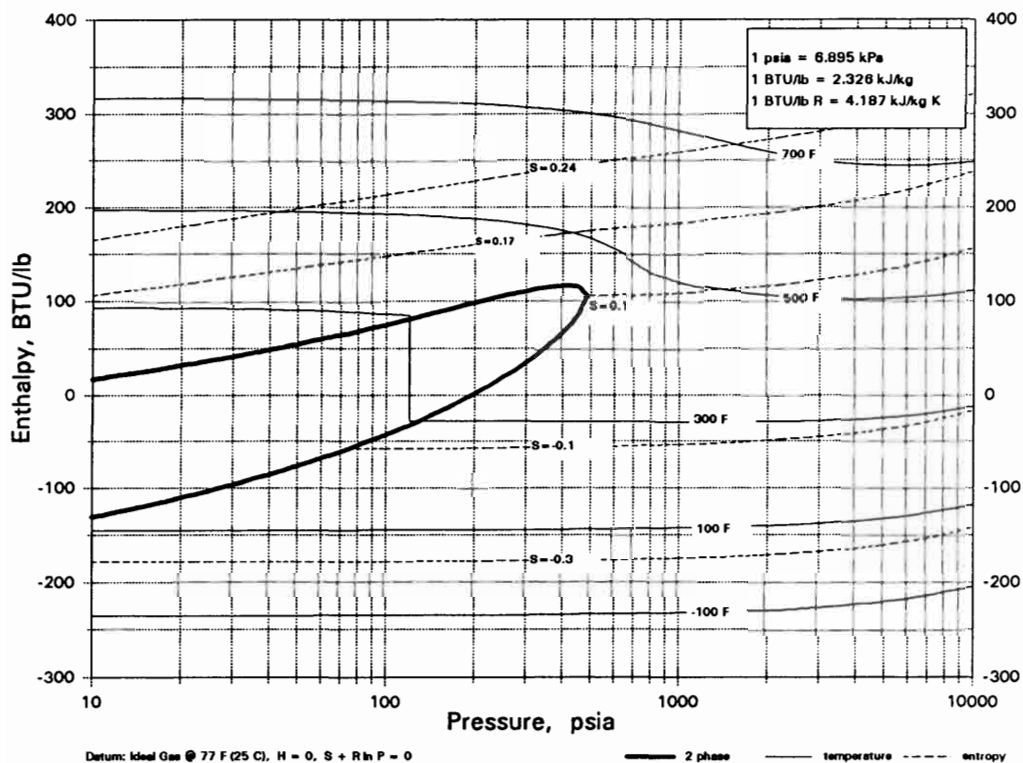
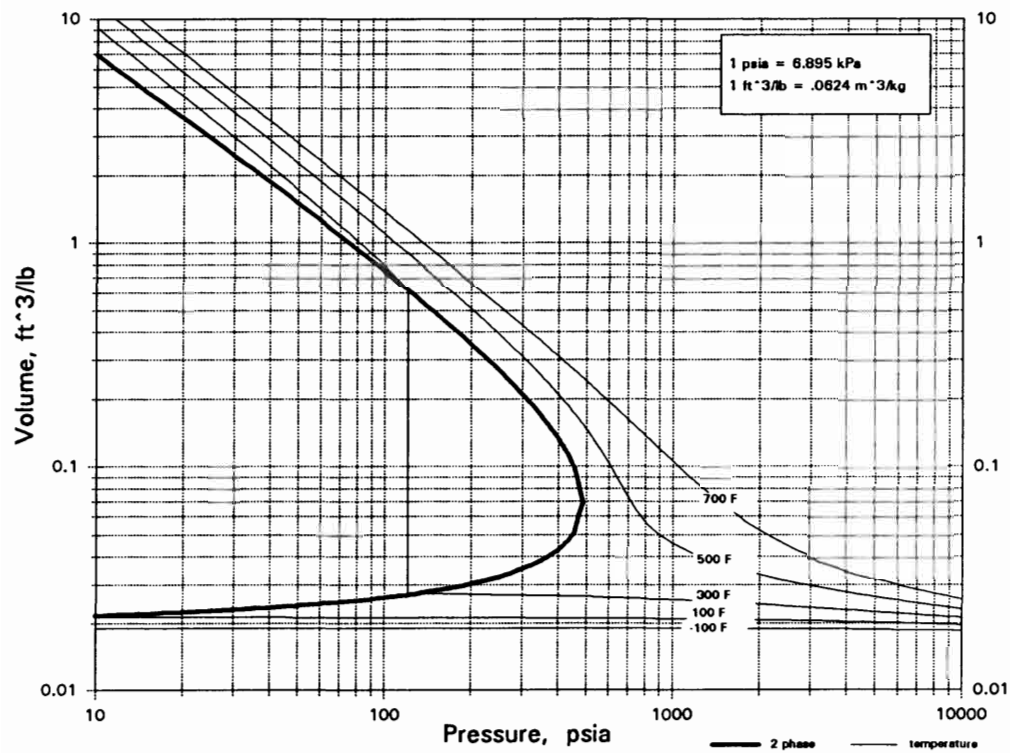
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METHYL ISOBUTYL ETHER



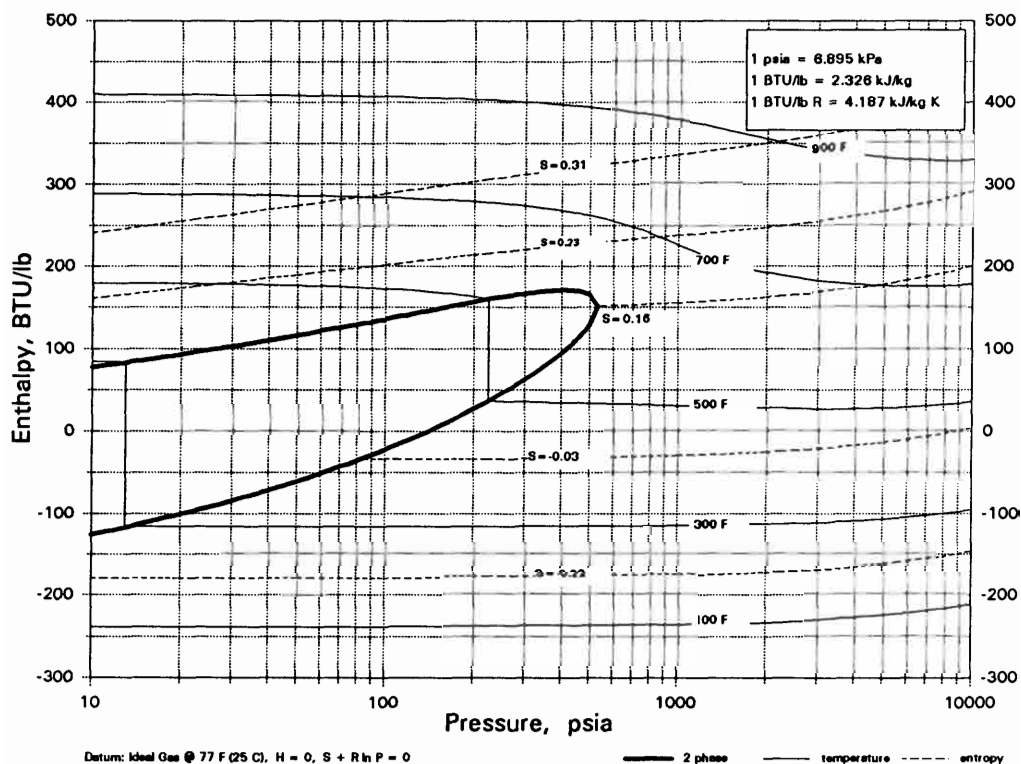
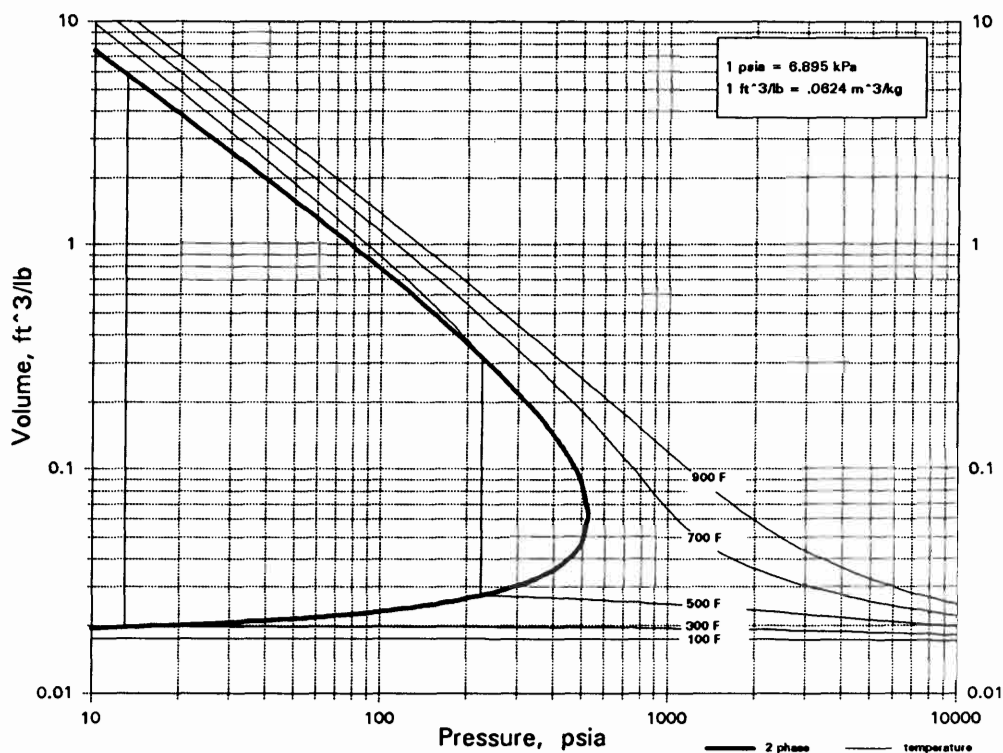
C5H12O

ETHYL PROPYL ETHER



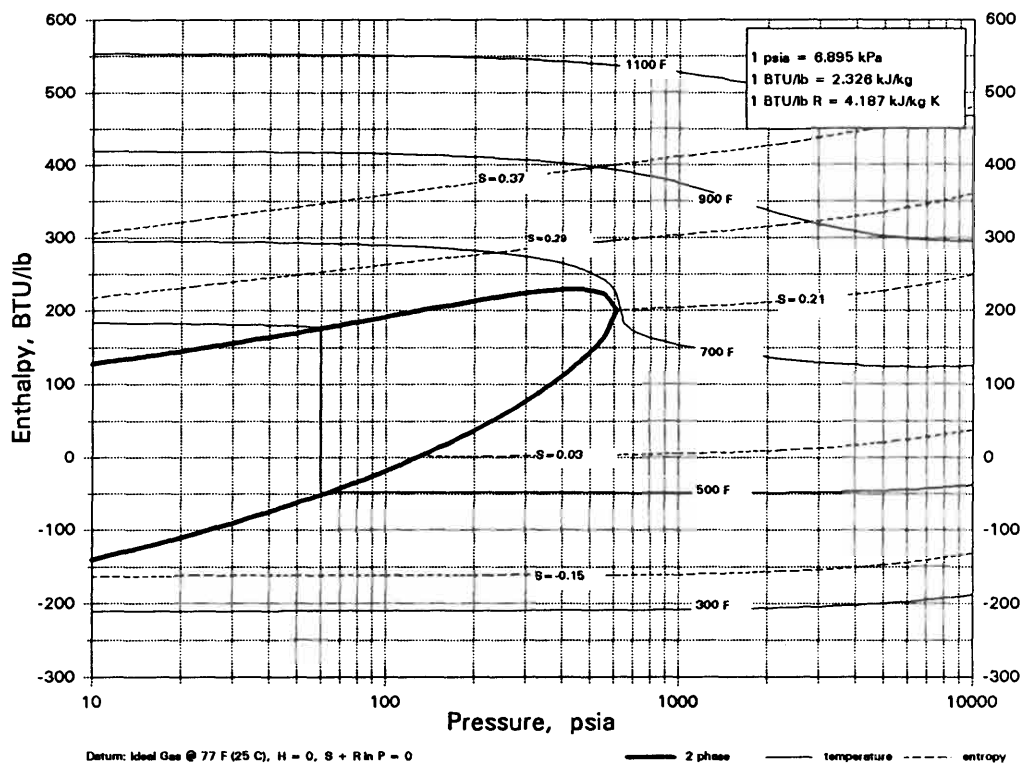
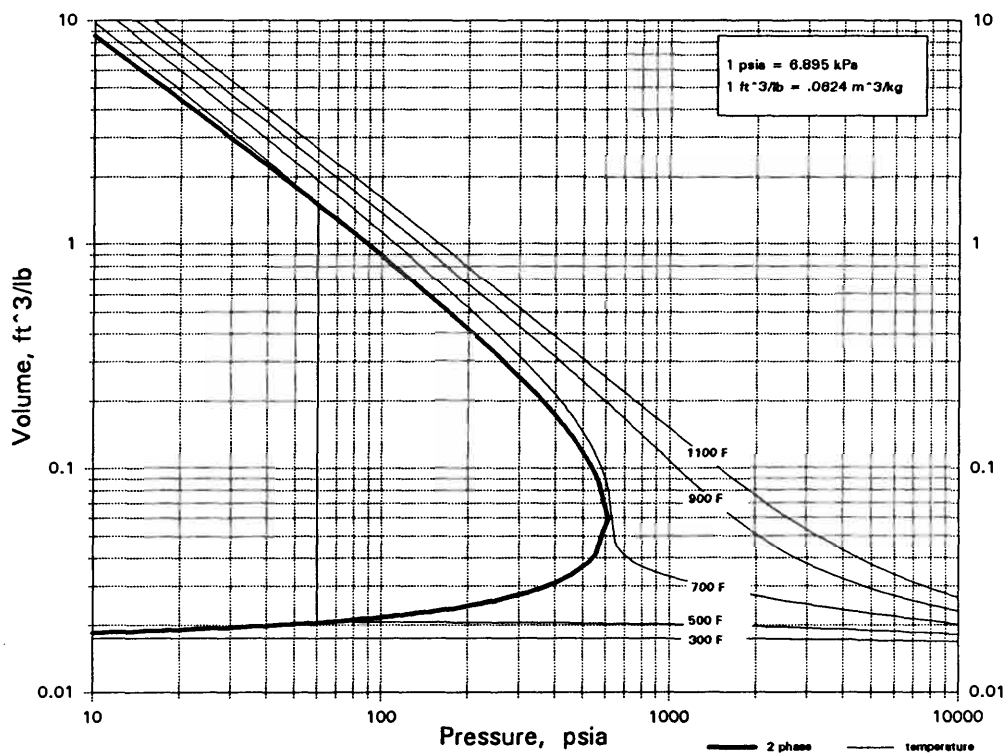
C5H12O2

ETHYLENE GLYCOL MONOPROPYL ETHER

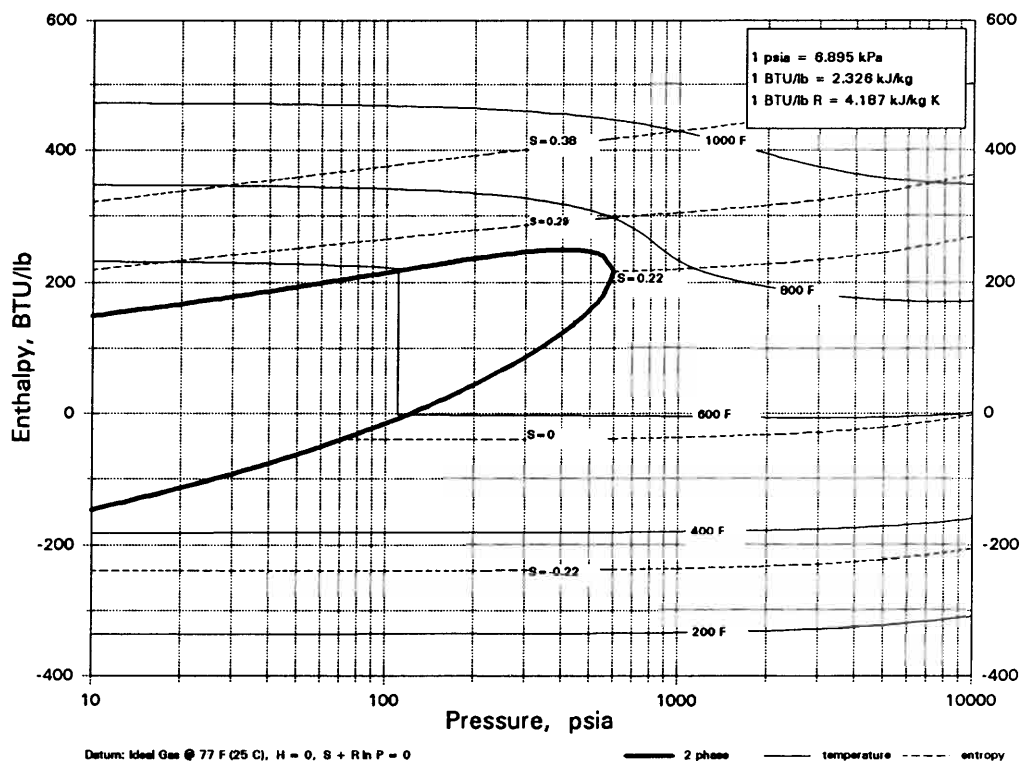
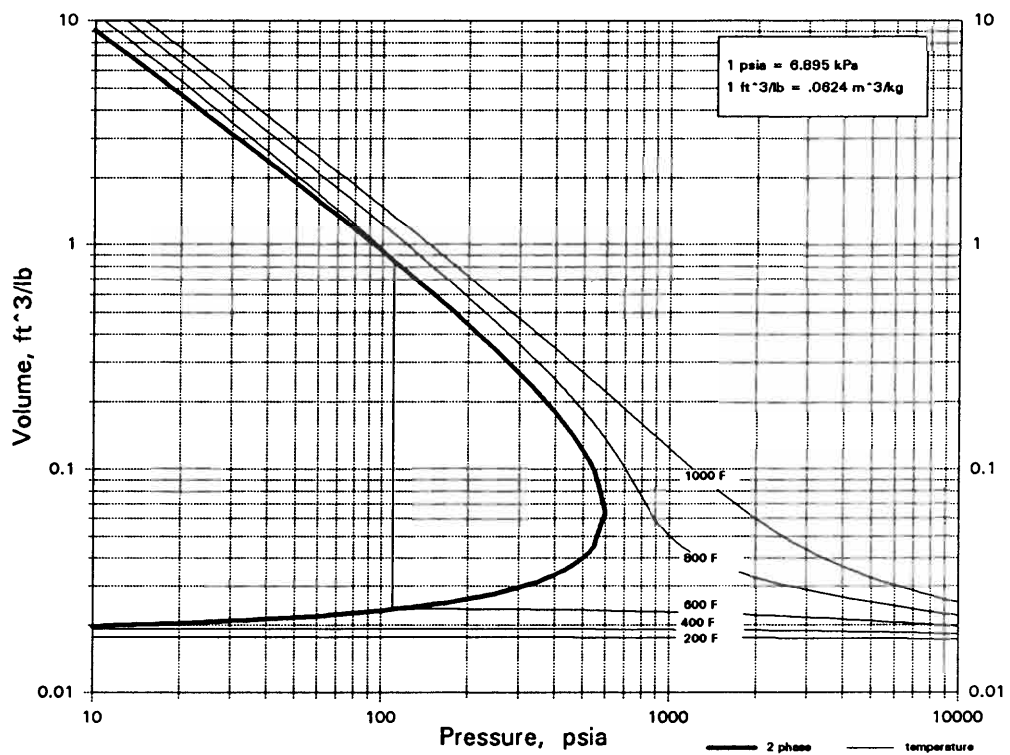


C5H12O2

NEOPENTYL GLYCOL

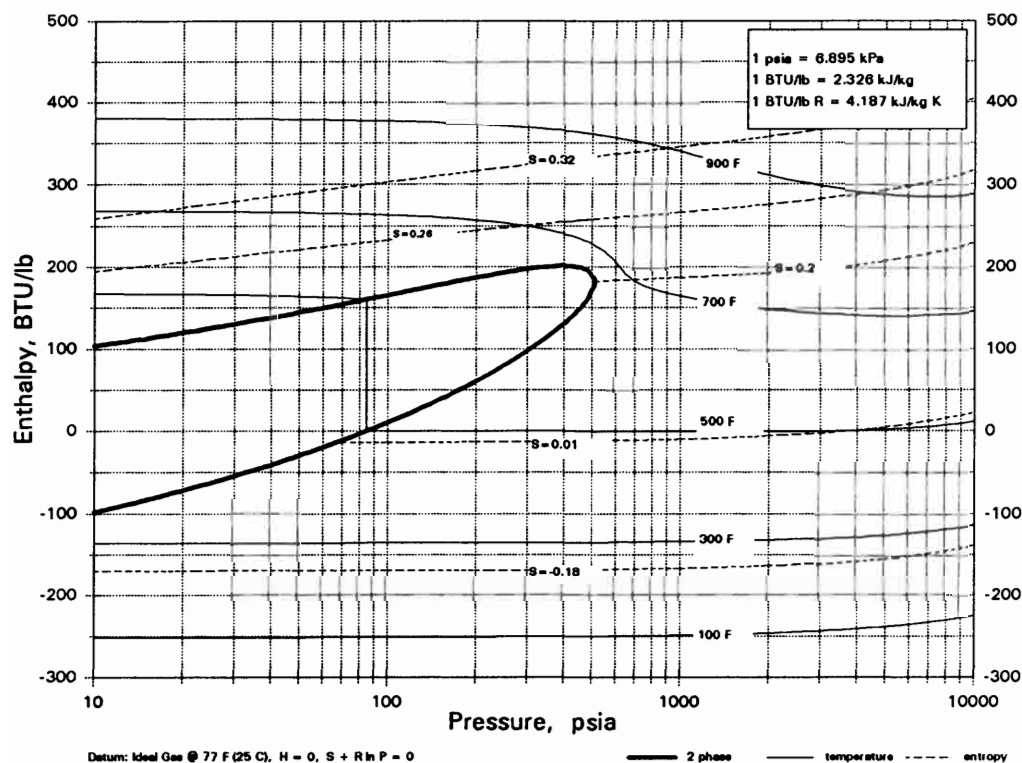
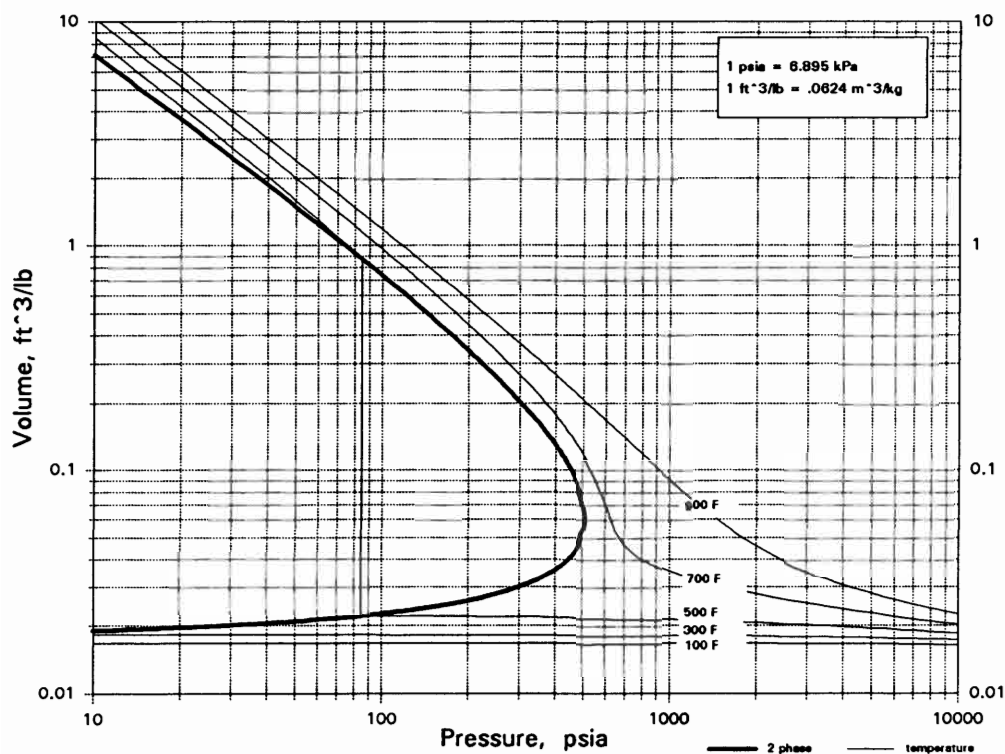


C5H12O2
1-5-PENTANEDIOL

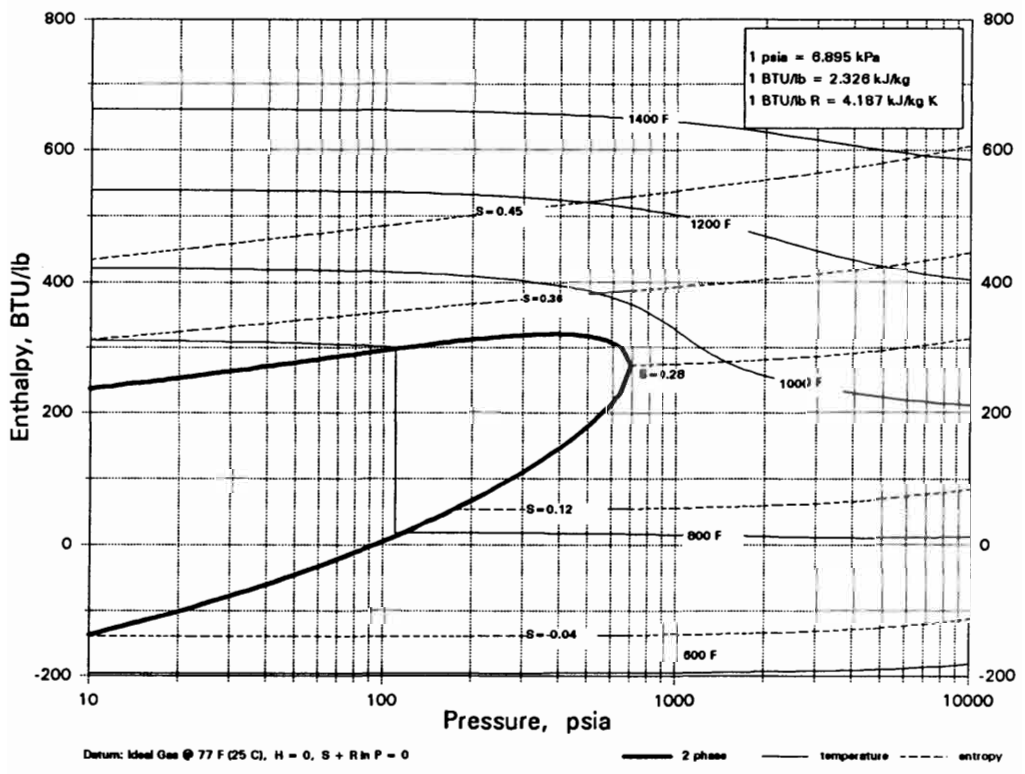
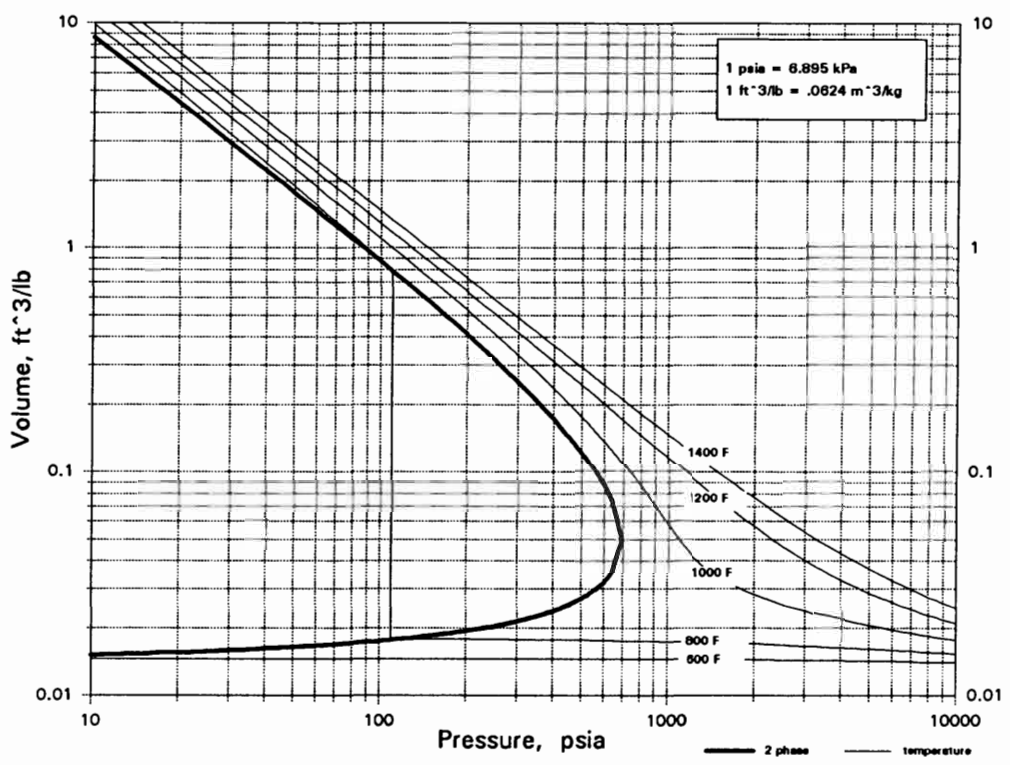


C5H12O3

2-(2-METHOXYETHOXY)ETHANOL

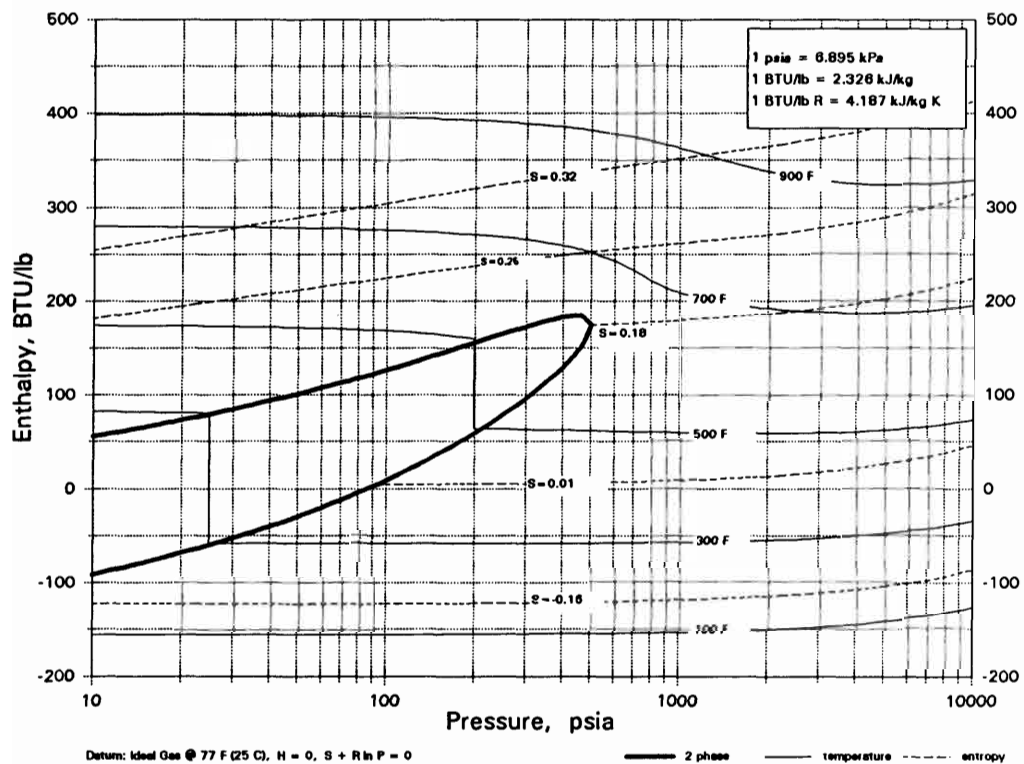
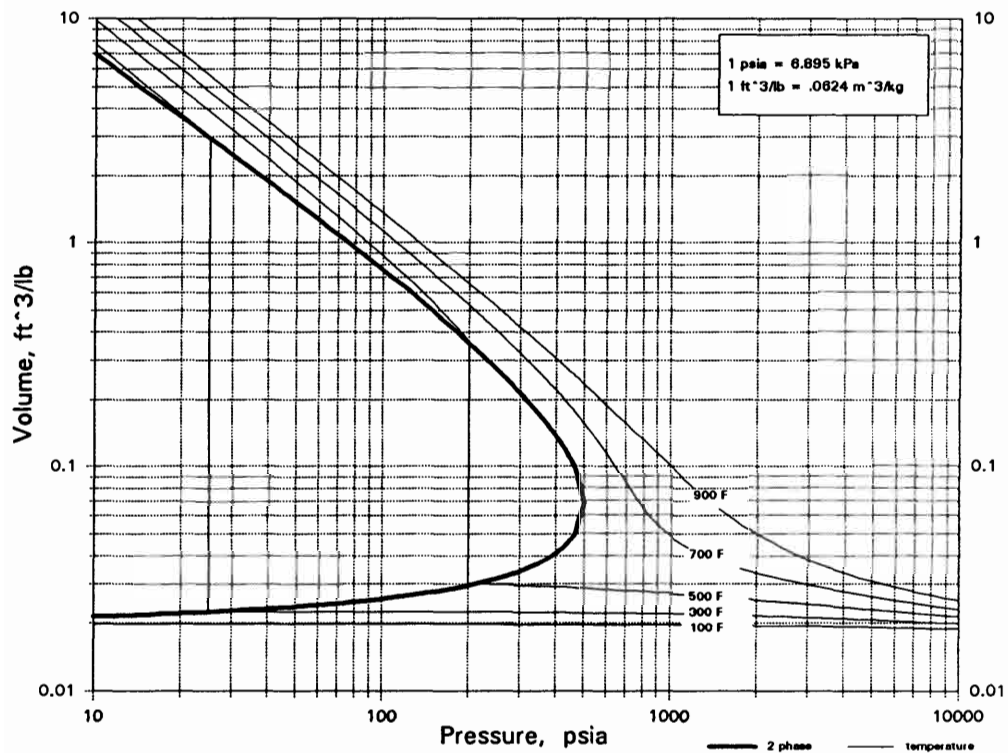


C5H12O4
PENTAERYTHRITOL



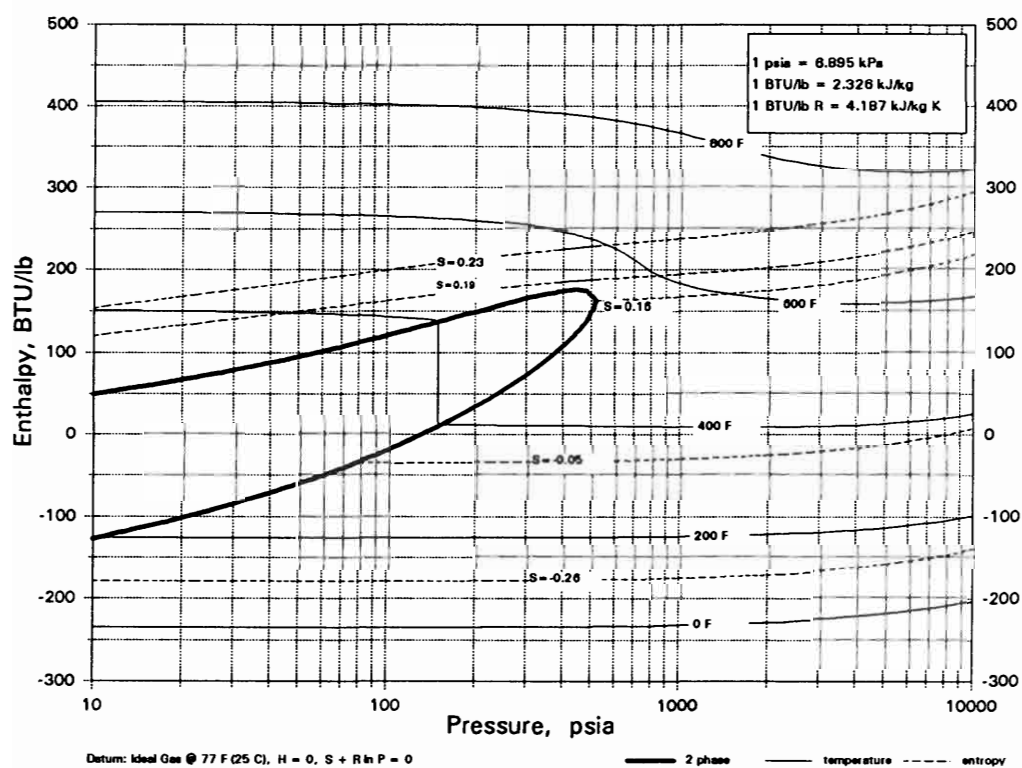
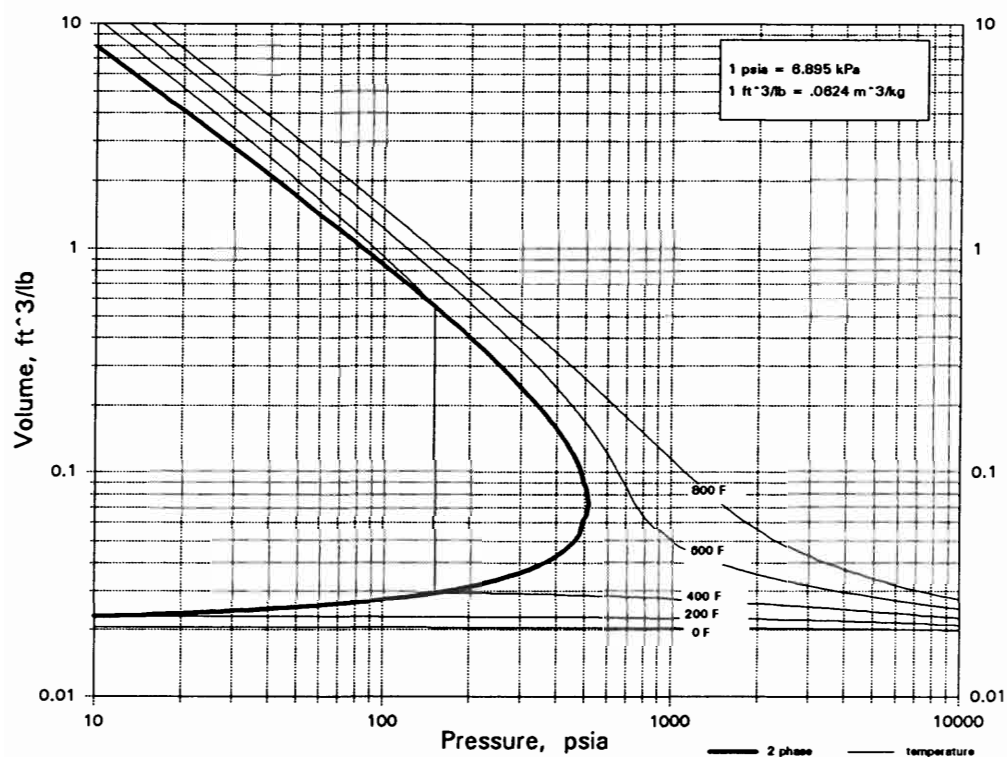
C5H12S

n-PENTYL MERCAPTAN



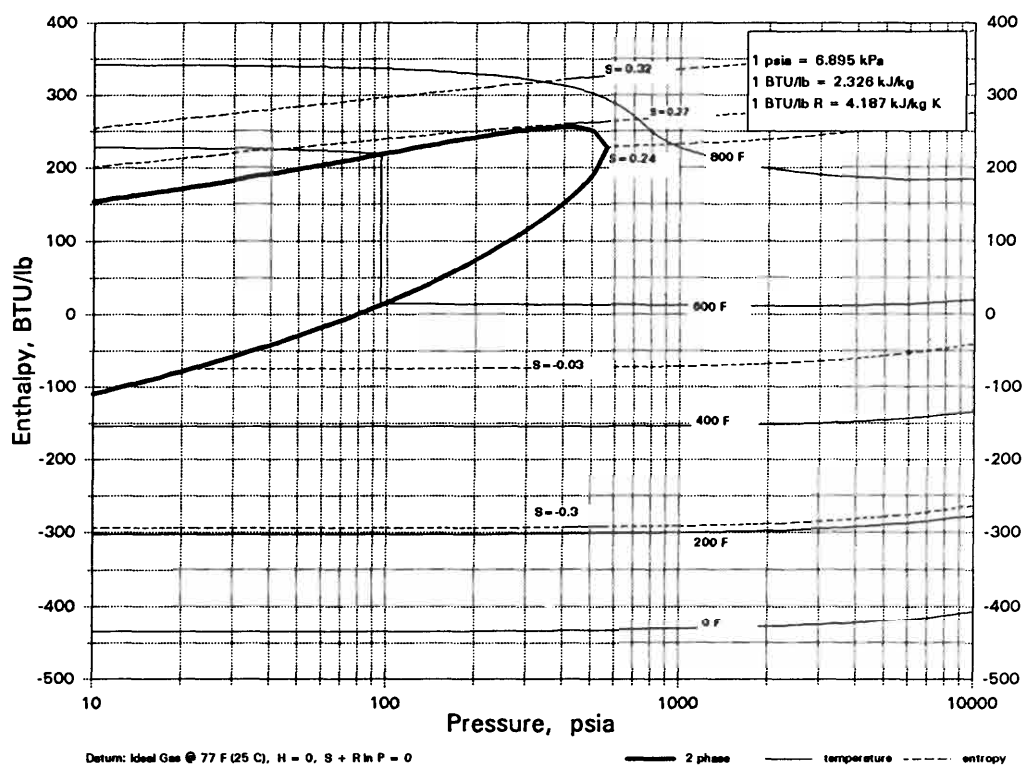
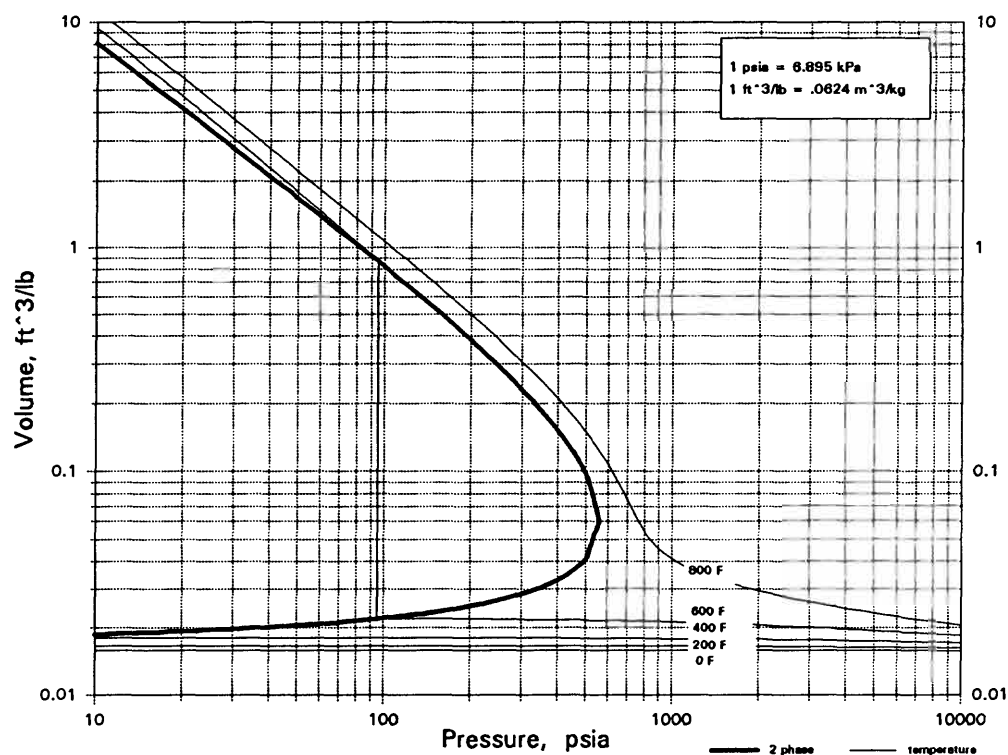
C5H13N

n-PENTYLAMINE

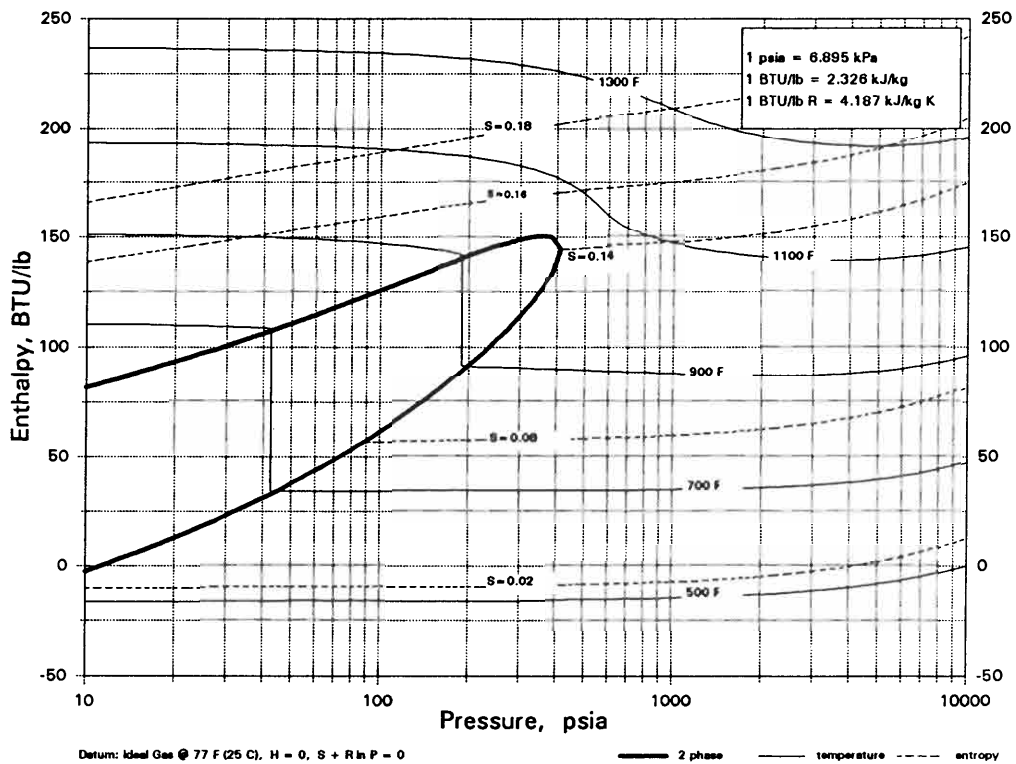
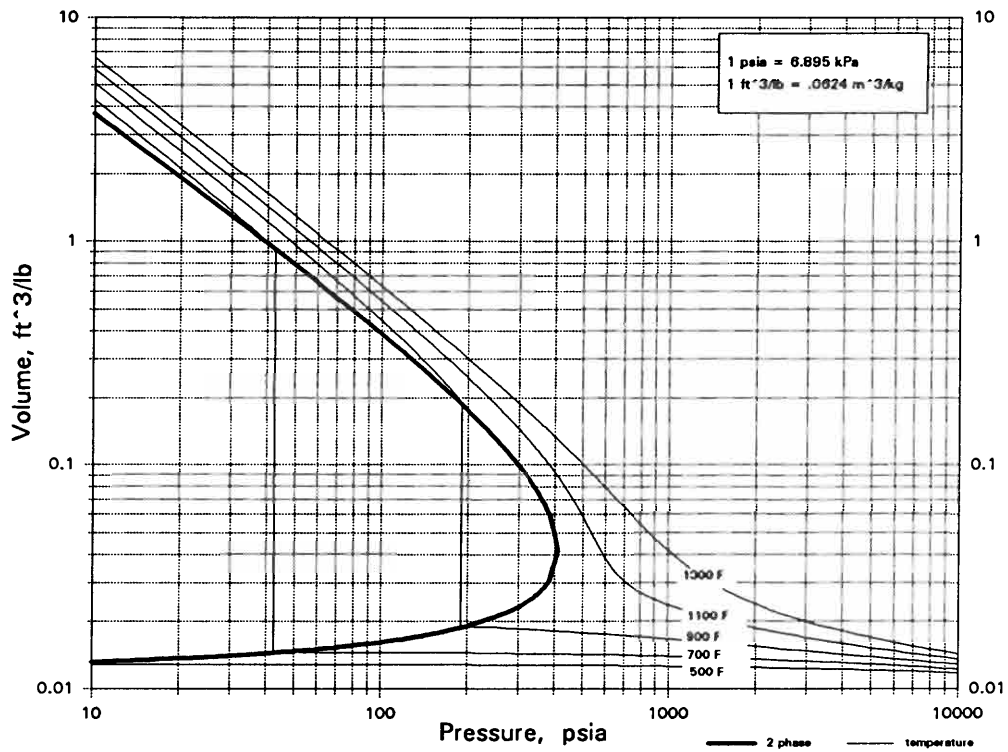


C5H13NO2

METHYL DIETHANOLAMINE

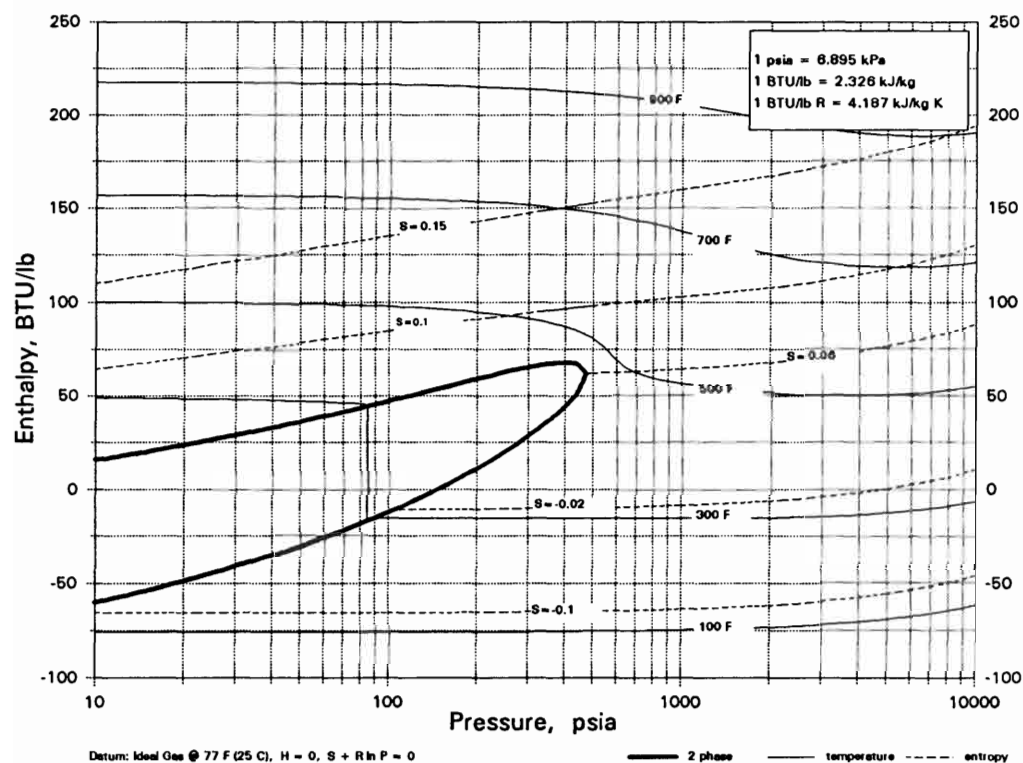
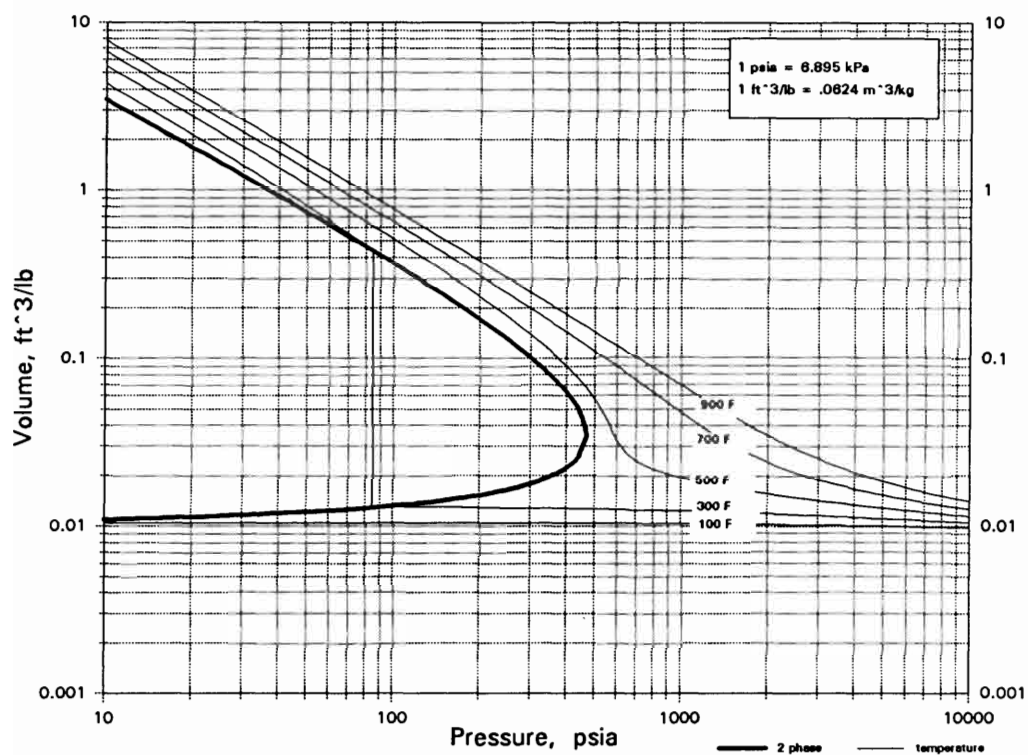


C6Cl6
HEXACHLOROBENZENE

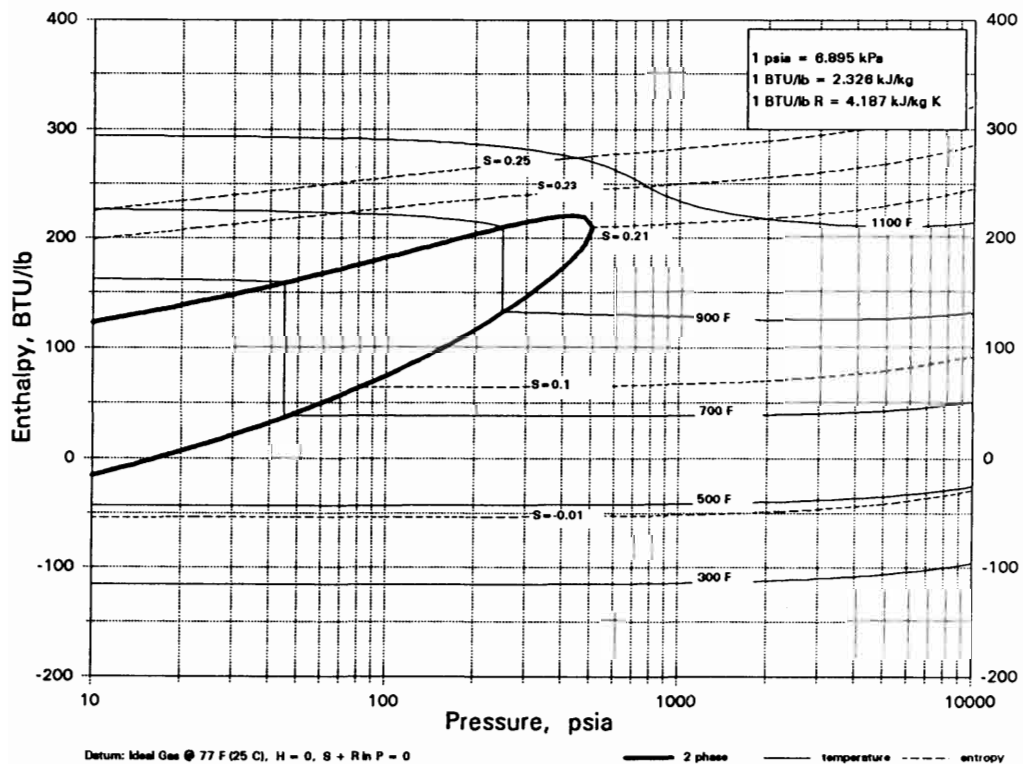
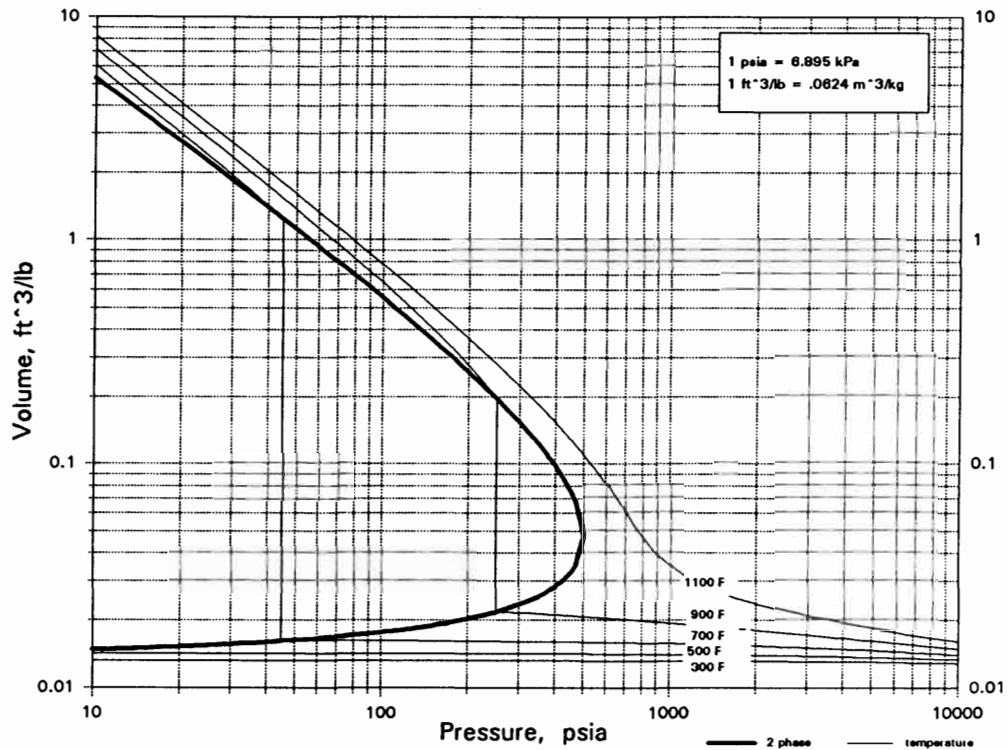


C6F6

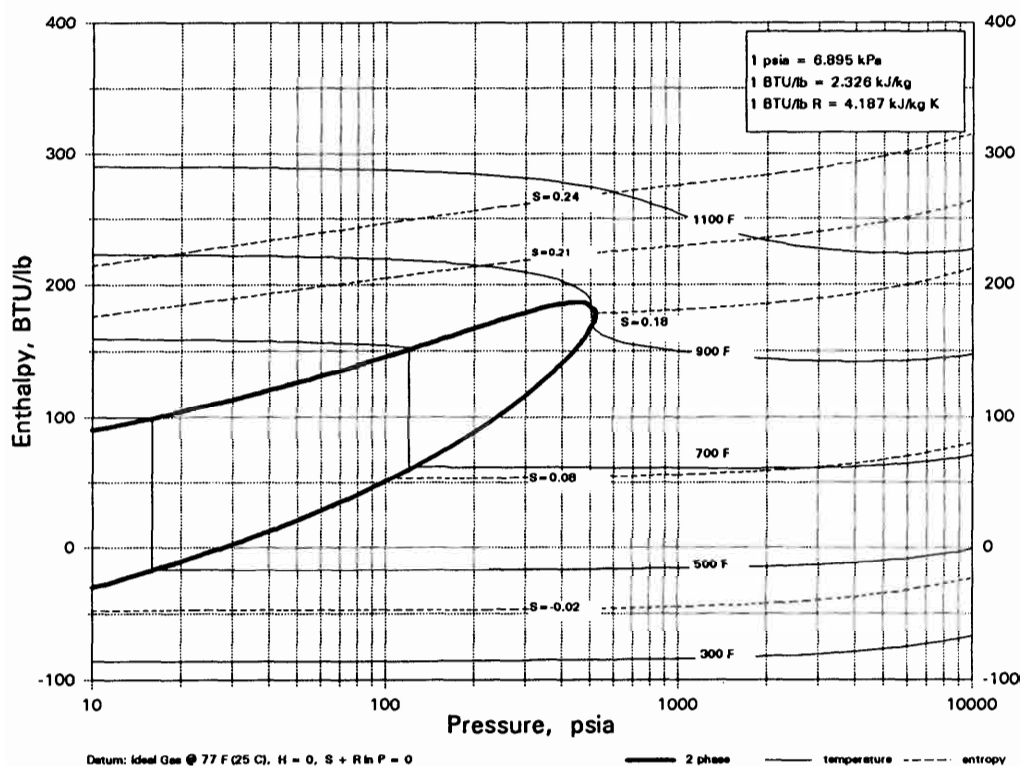
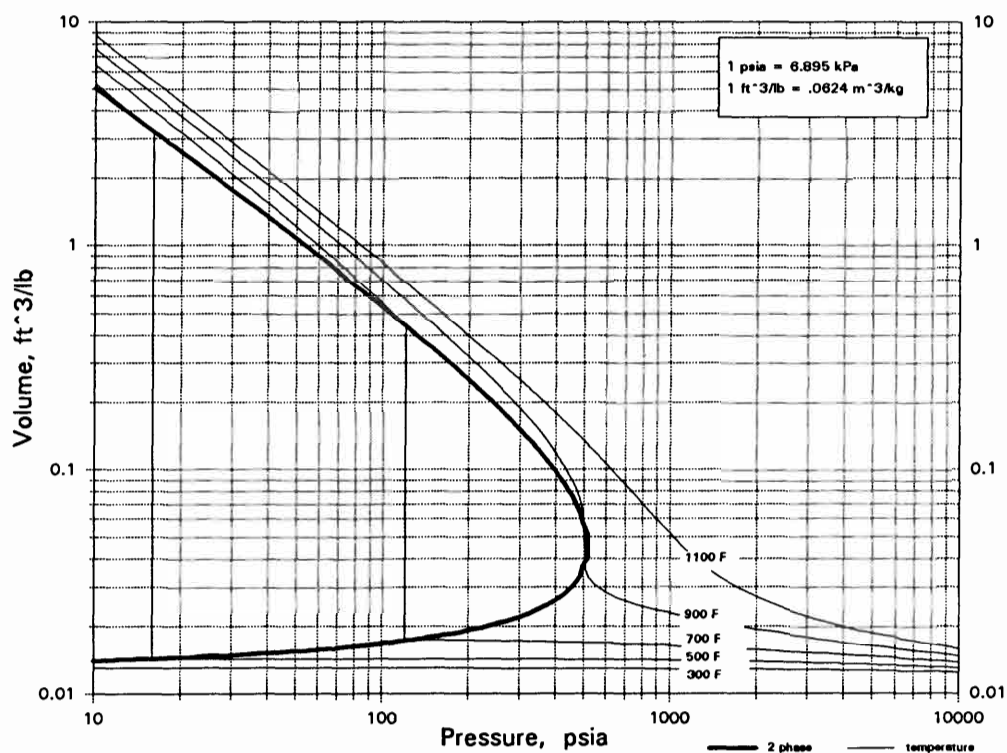
HEXAFLUOROBENZENE



C6H3ClN2O4 1-CHLORO-2,4-DINITROBENZENE

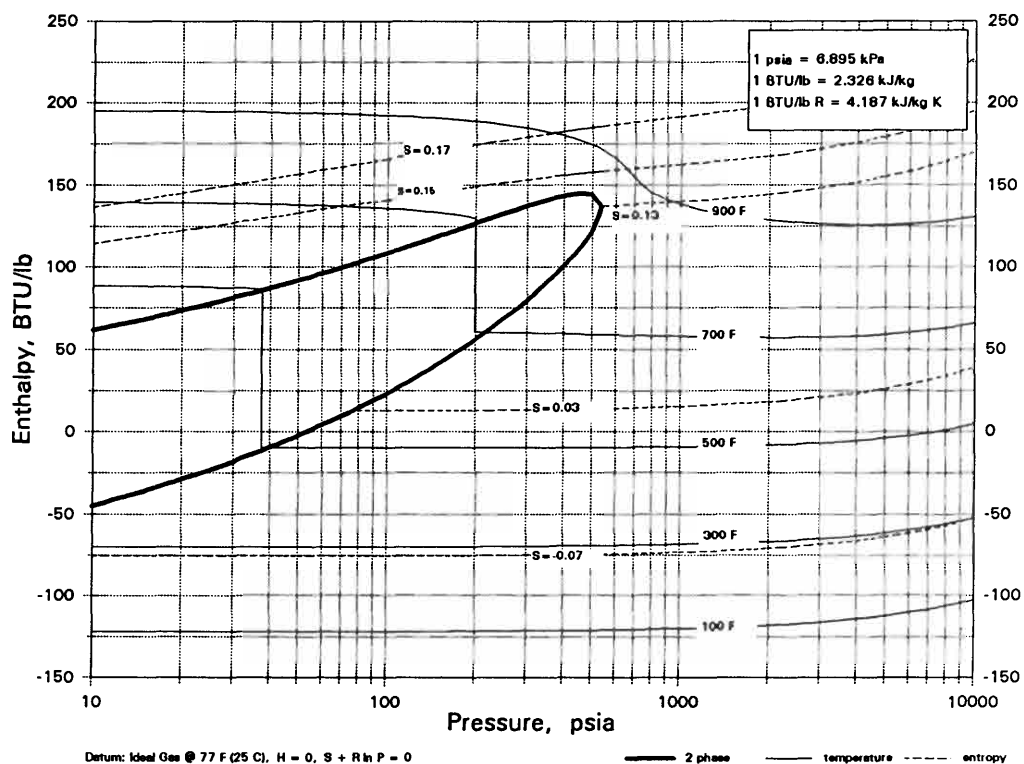
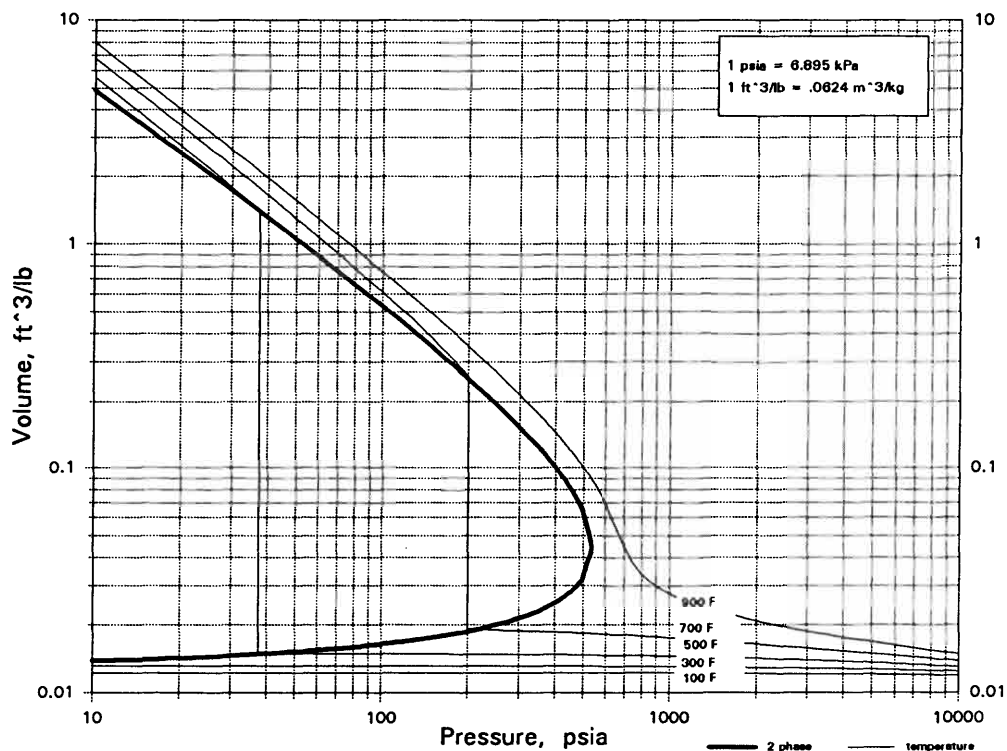


C6H3Cl2NO2 1-2-DICHLORO-4-NITROBENZENE



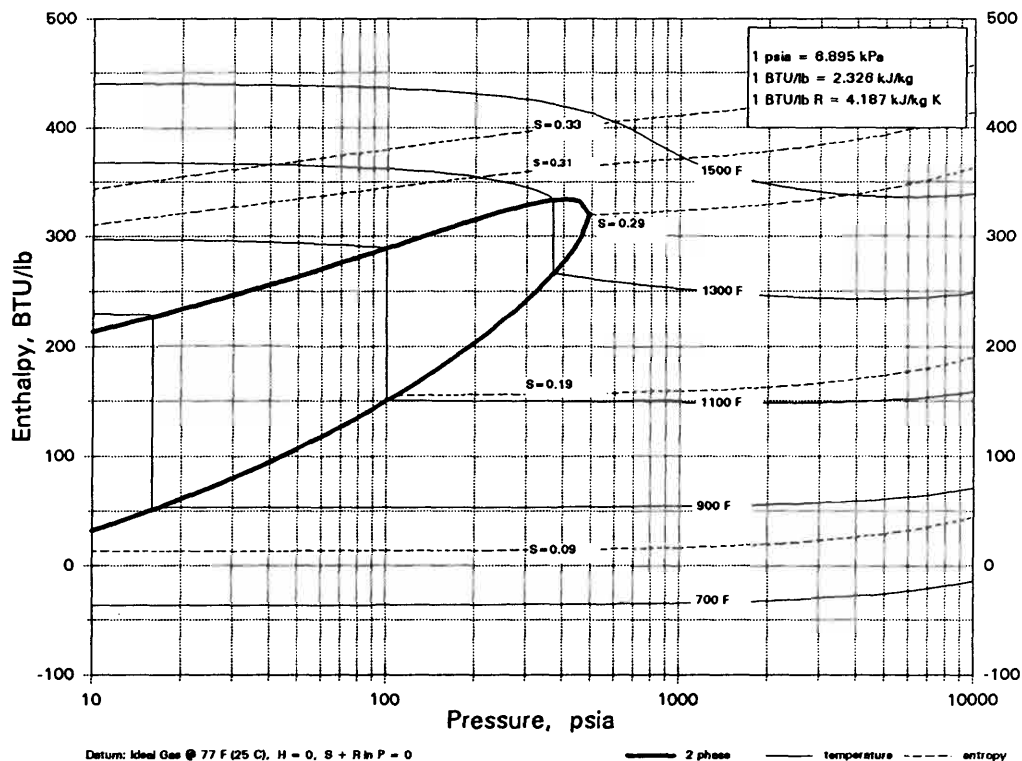
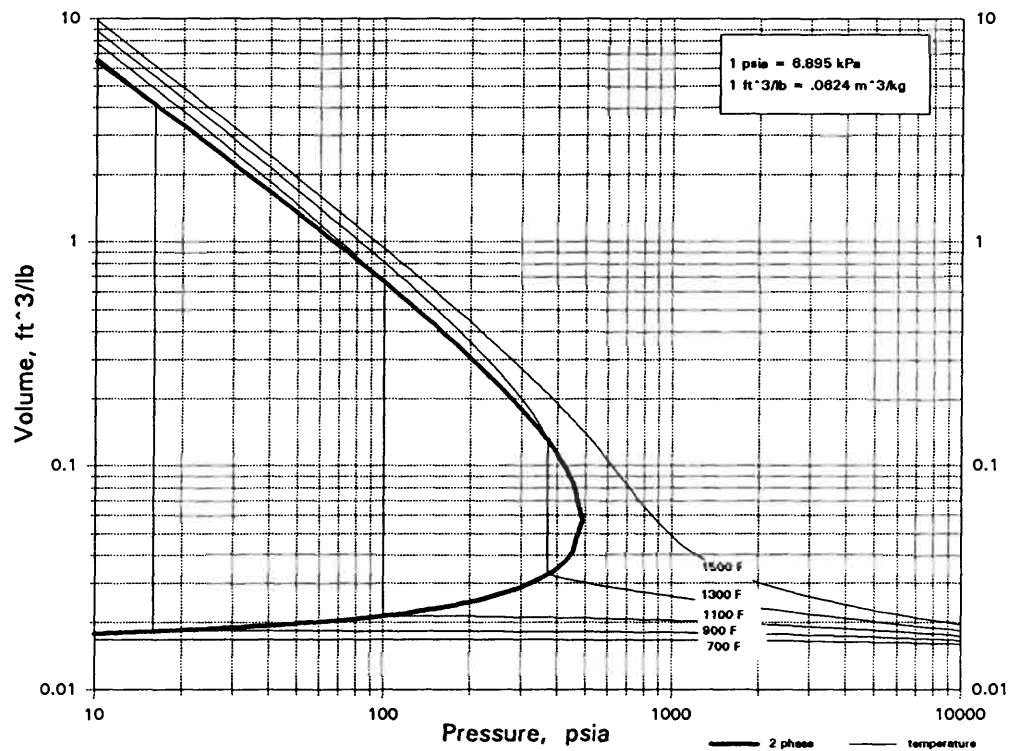
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1-2-4-TRICHLOROBENZENE



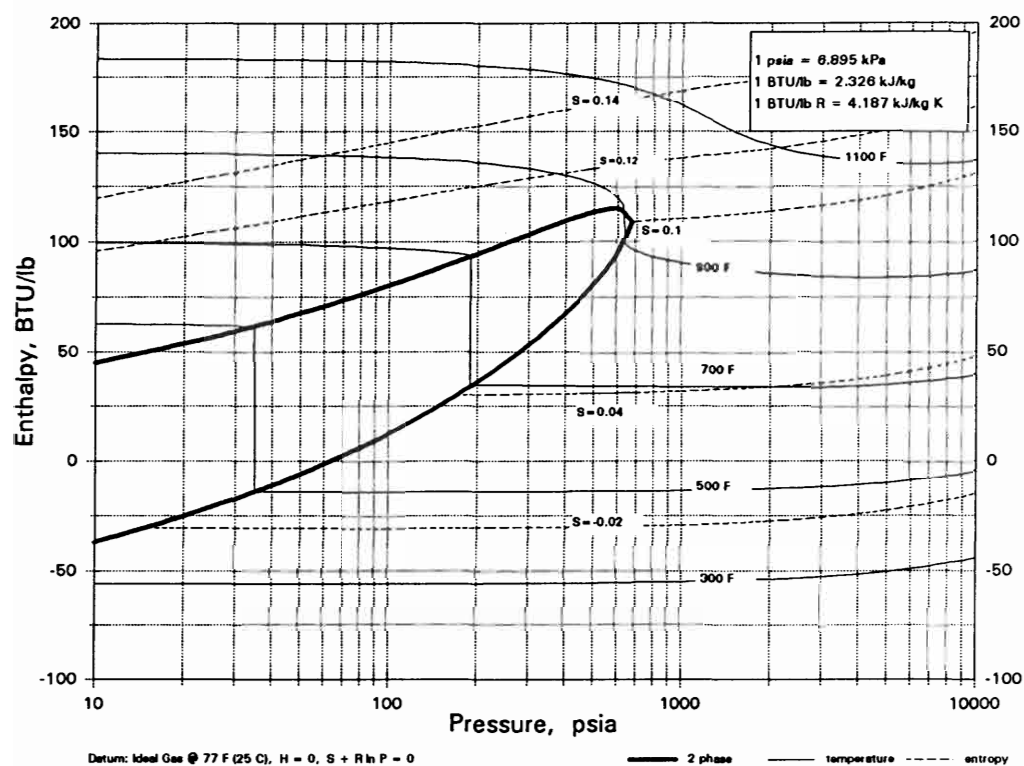
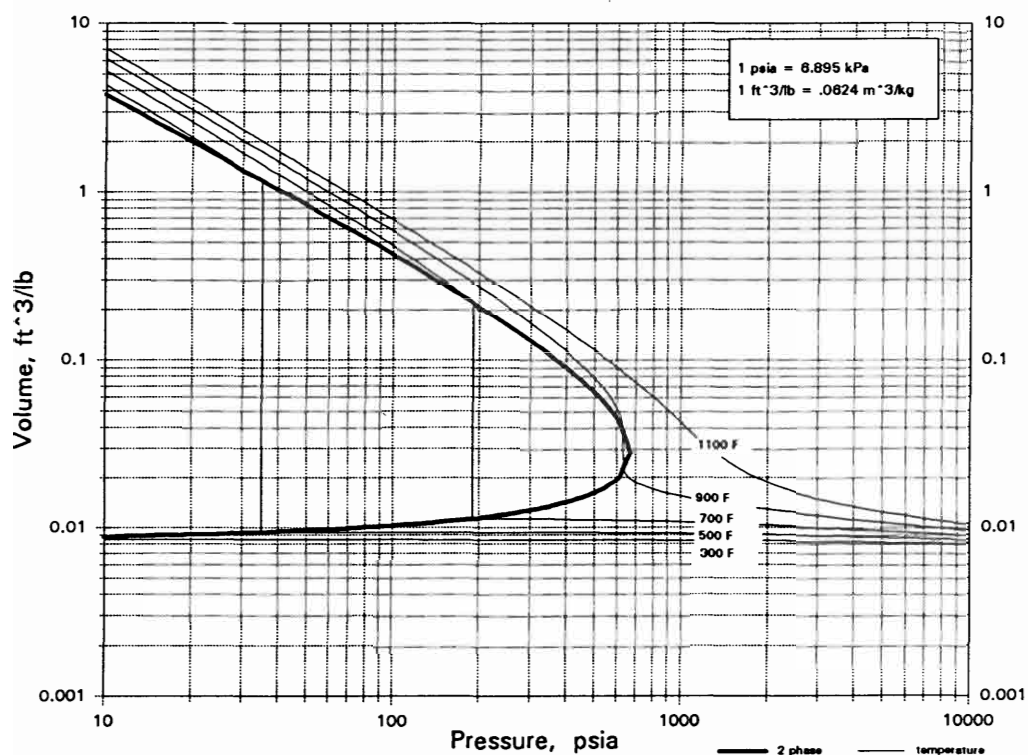
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1-3-5-TRINITROBENZENE

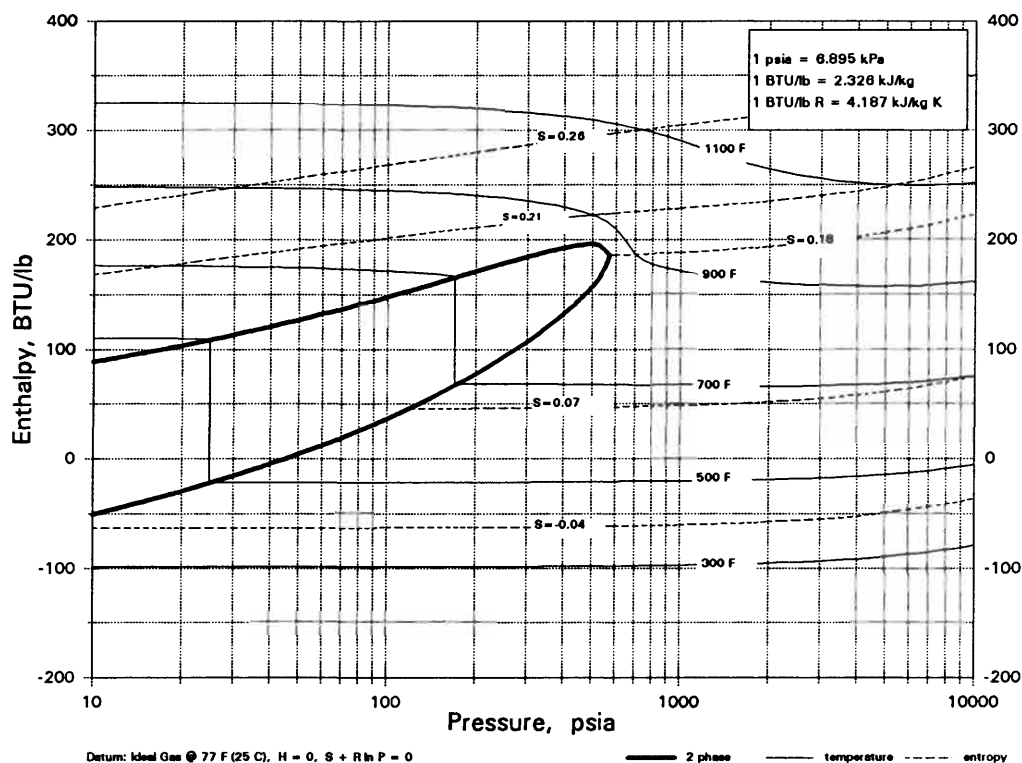
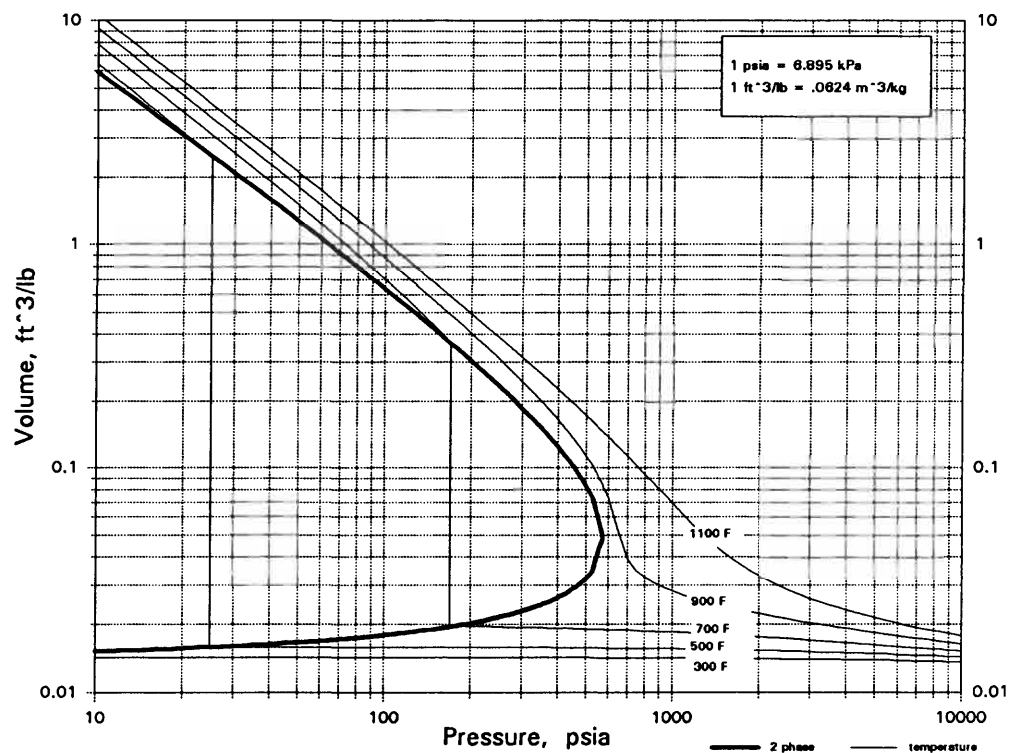


C6H4Br2

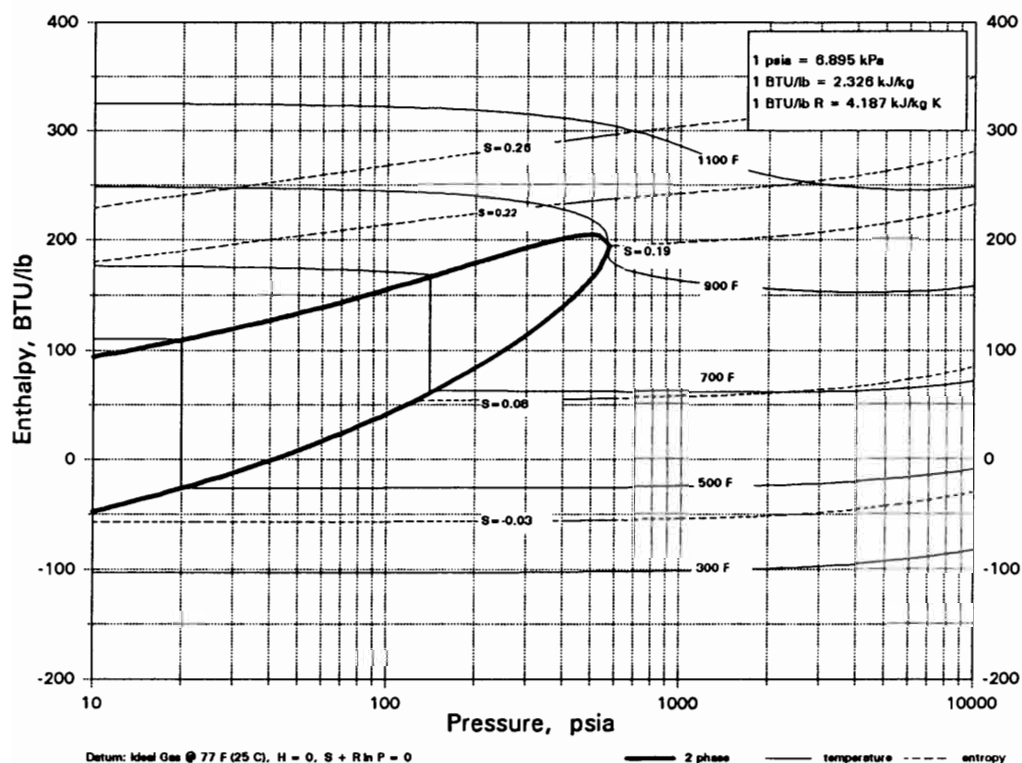
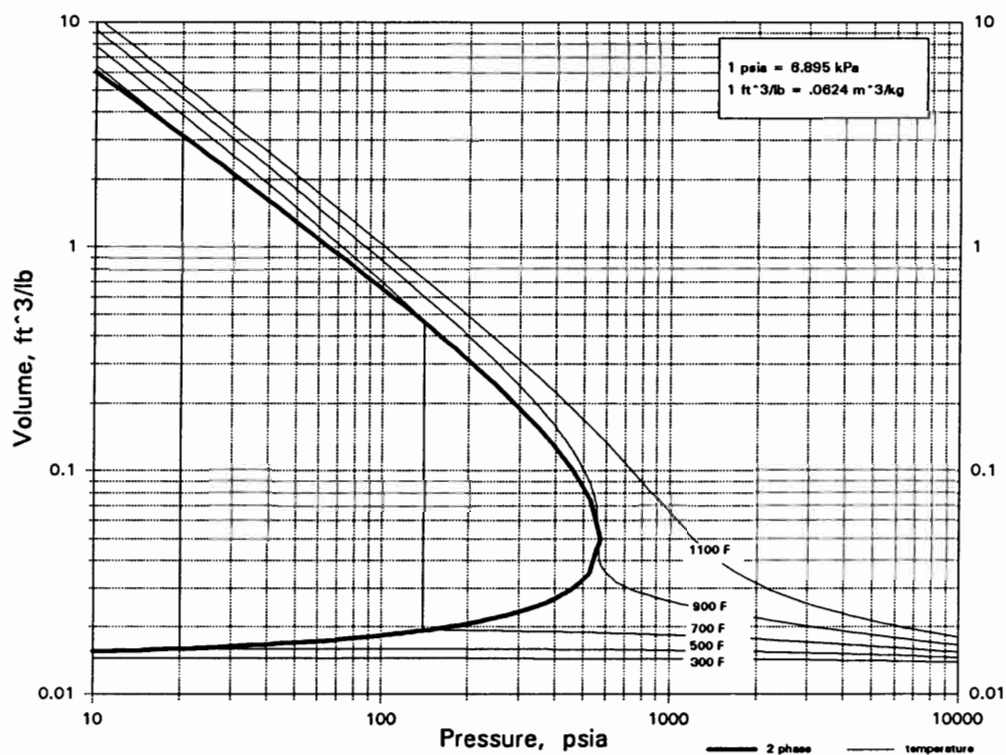
m-DIBROMOBENZENE



C6H4ClNO2 m-CHLORONITROBENZENE

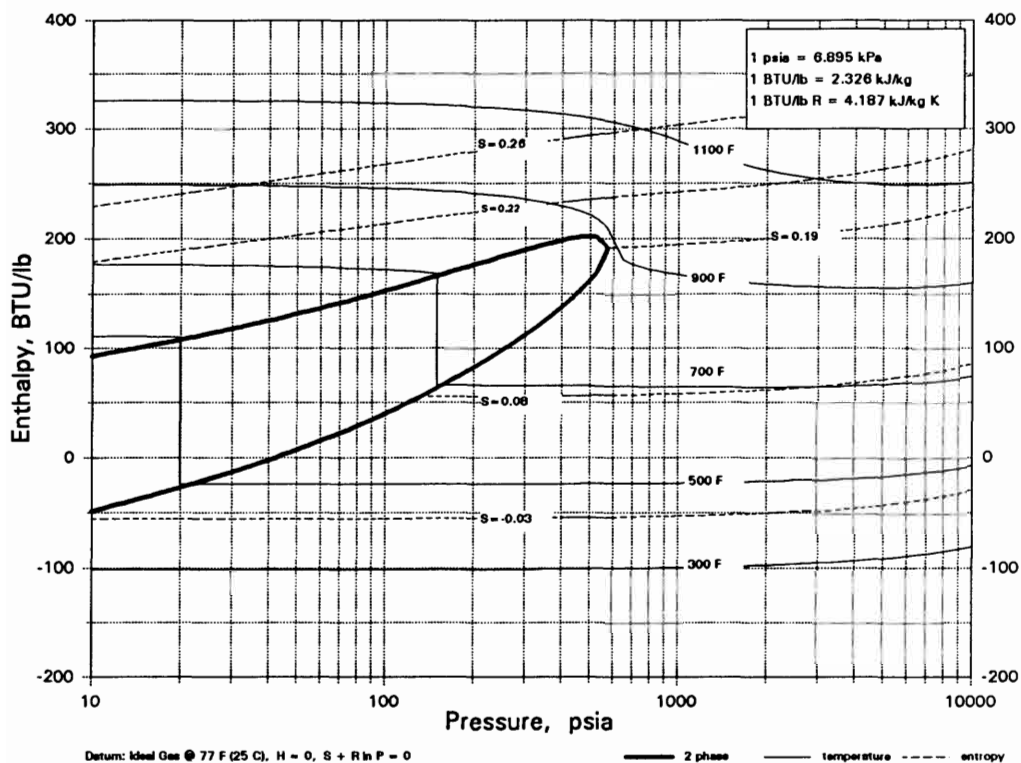
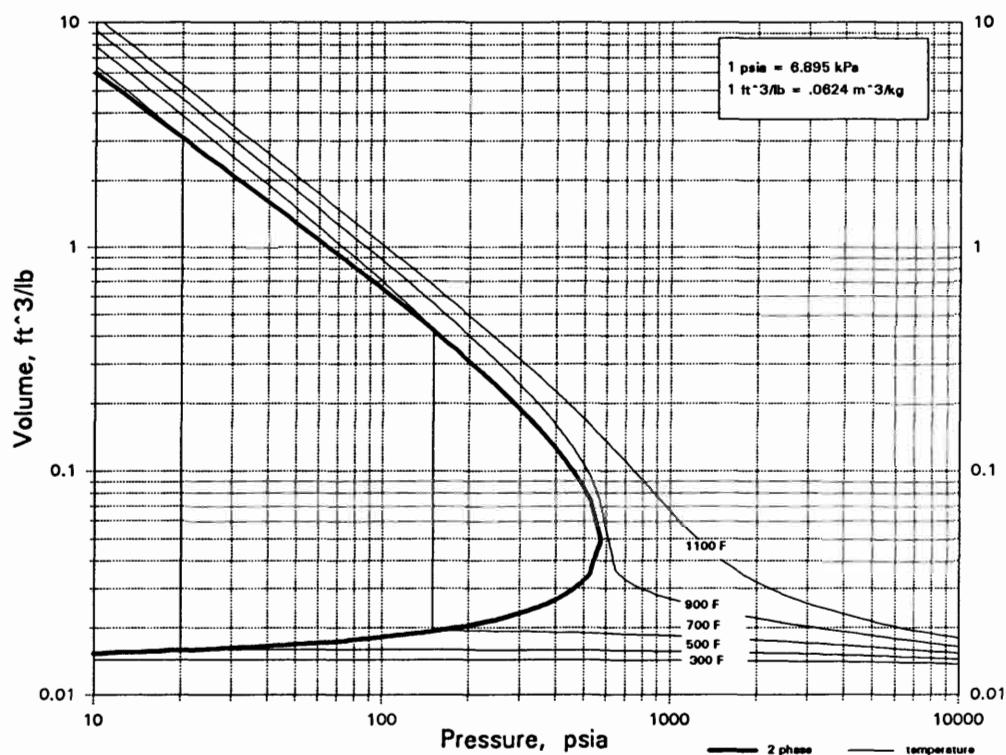


C₆H₄ClNO₂ o-CHLORONITROBENZENE

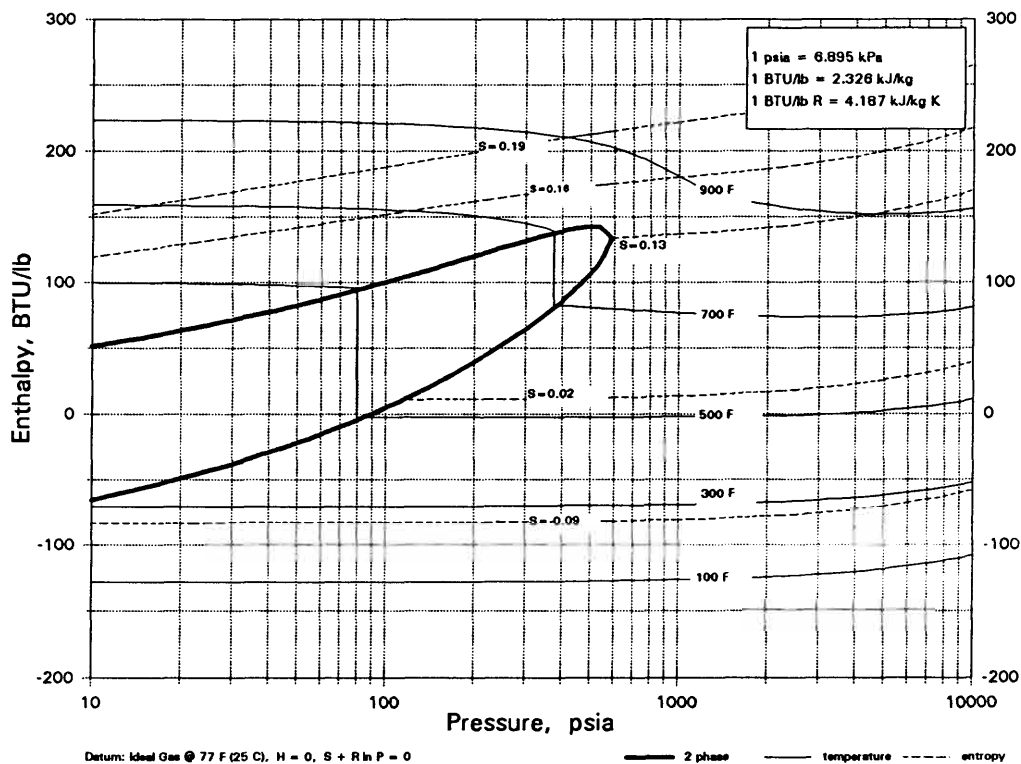
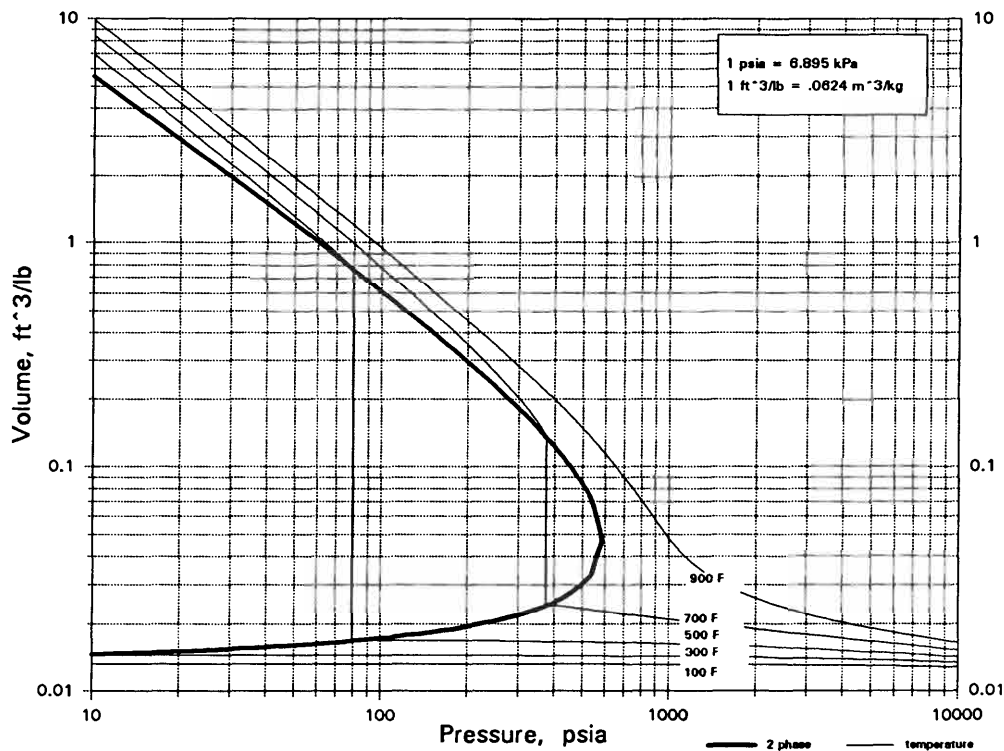


C6H4ClNO2

p-CHLORONITROBENZENE

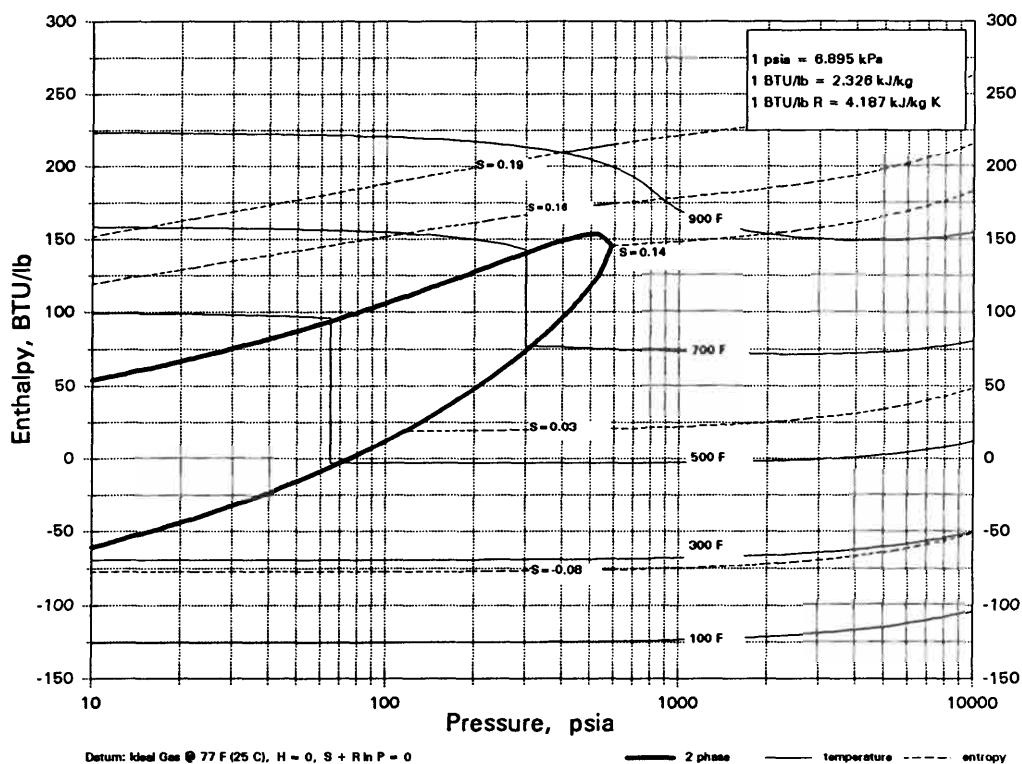
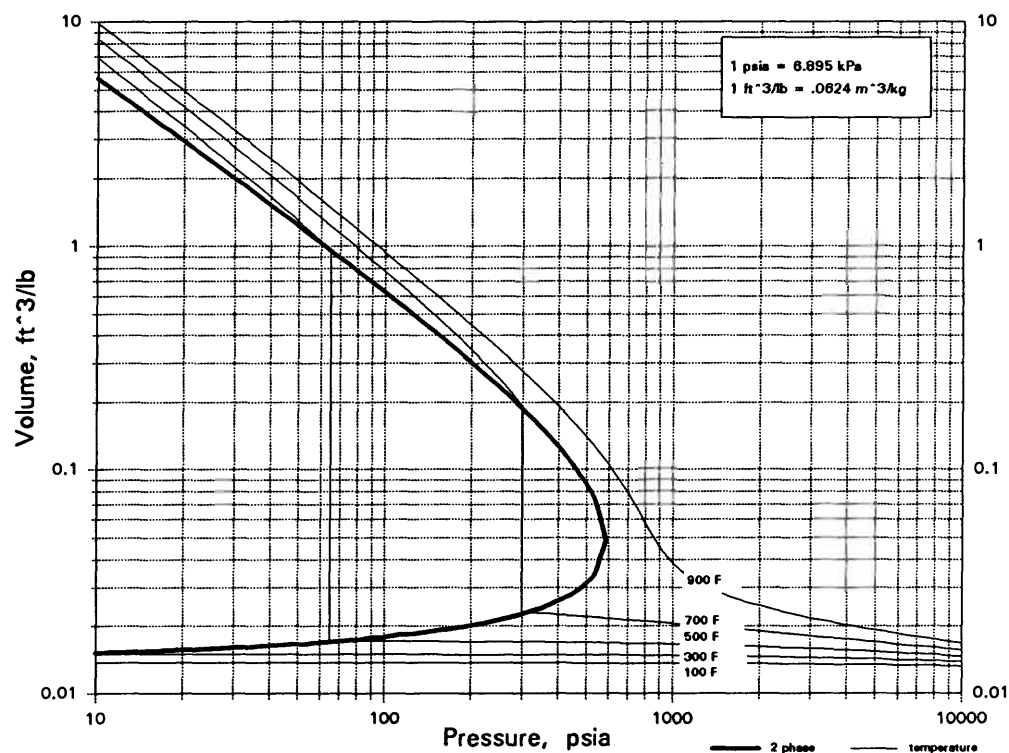


C6H4Cl2
m-DICHLOROBENZENE



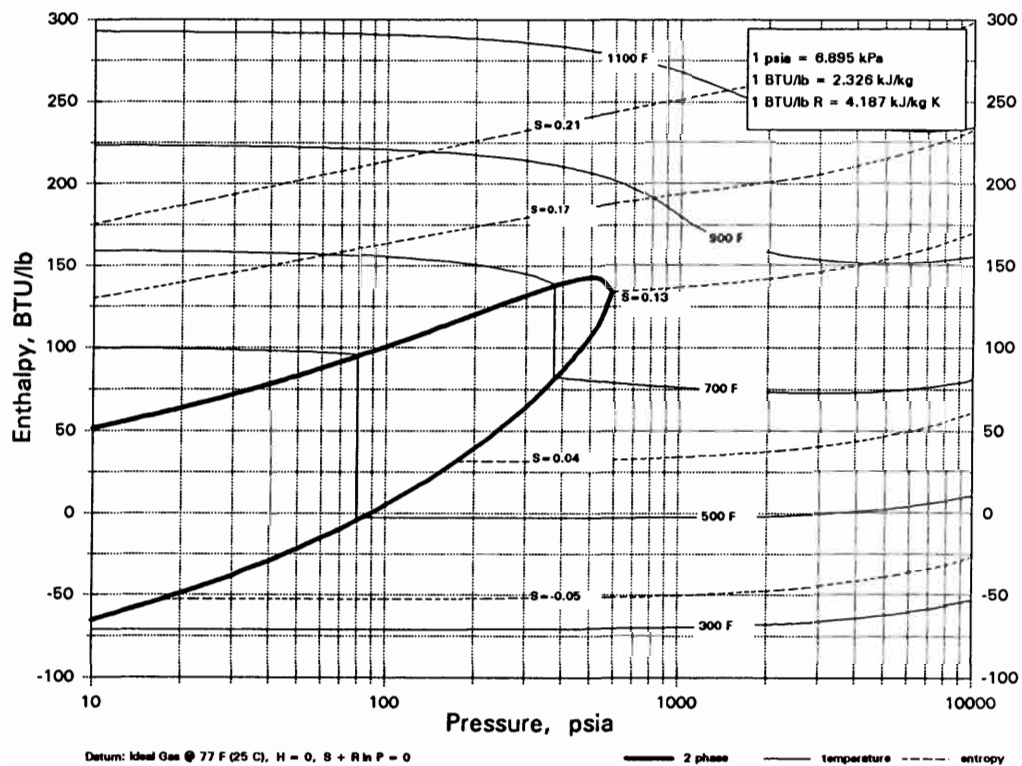
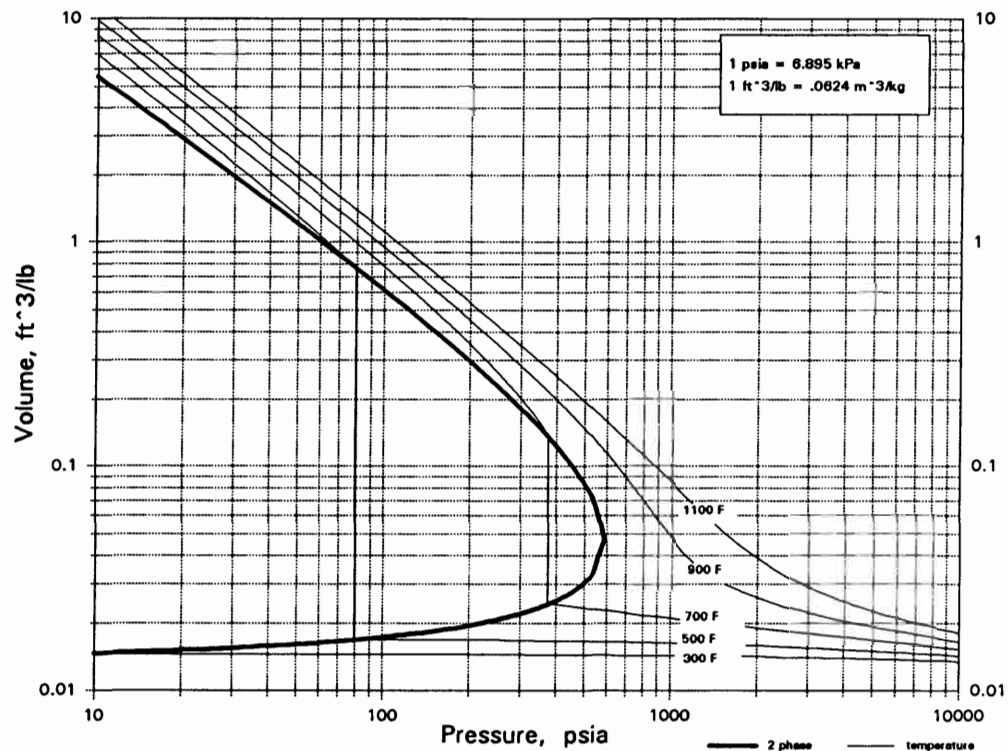
C6H4Cl2

o-DICHLOROBENZENE



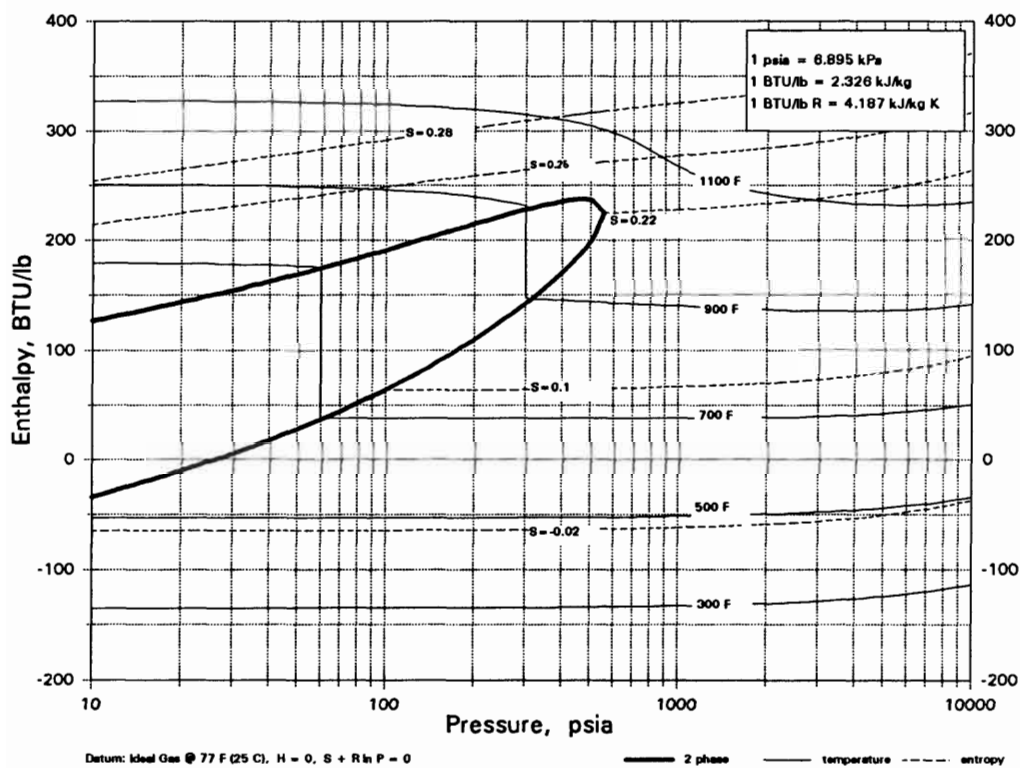
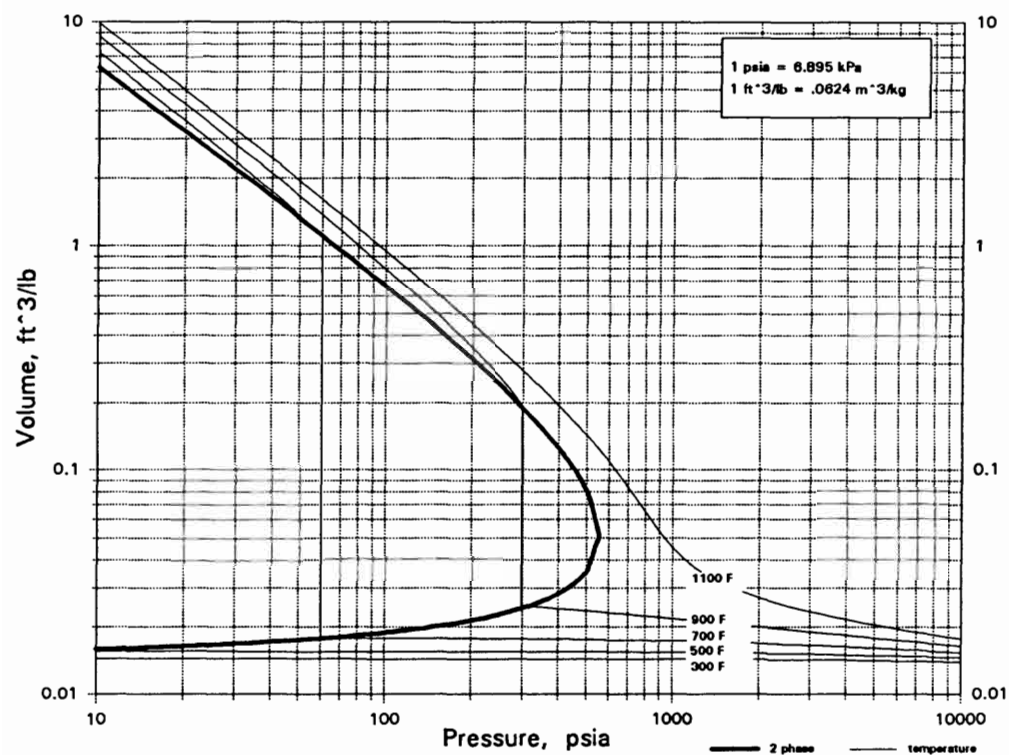
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p-DICHLOROBENZENE



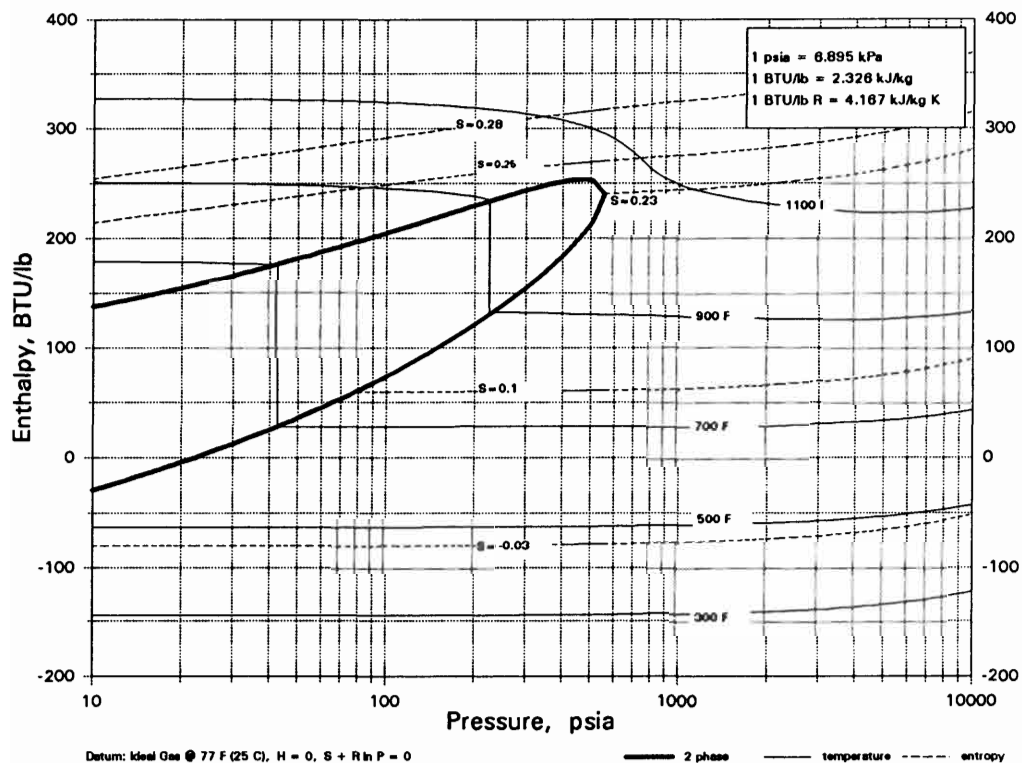
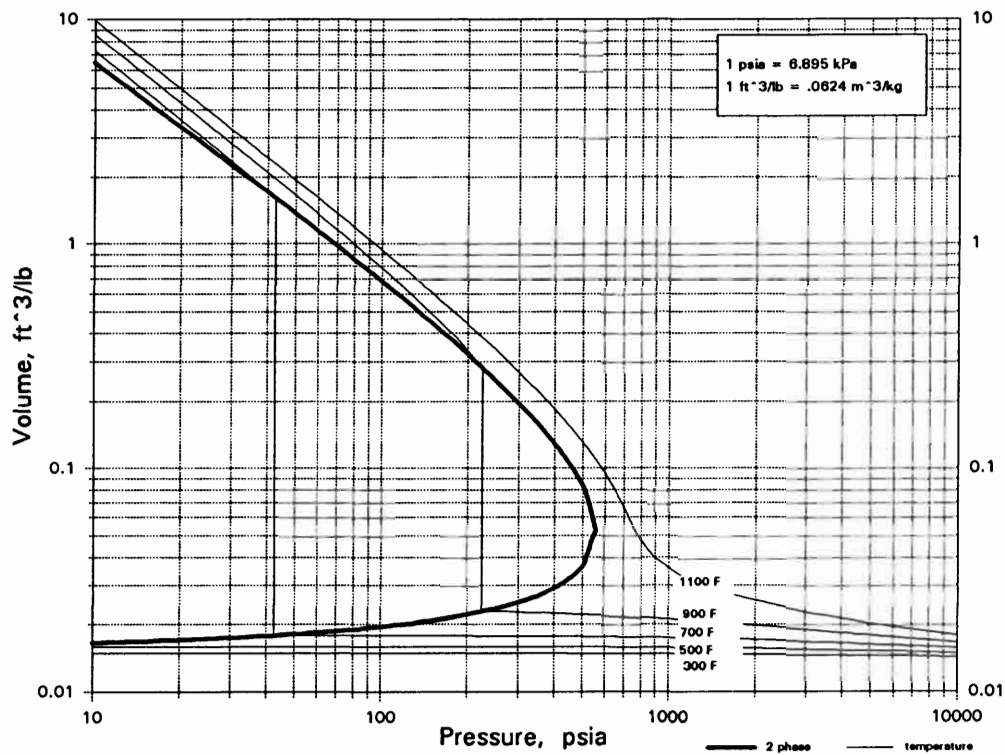
C₆H₄N₂O₄

m-DINITROBENZENE



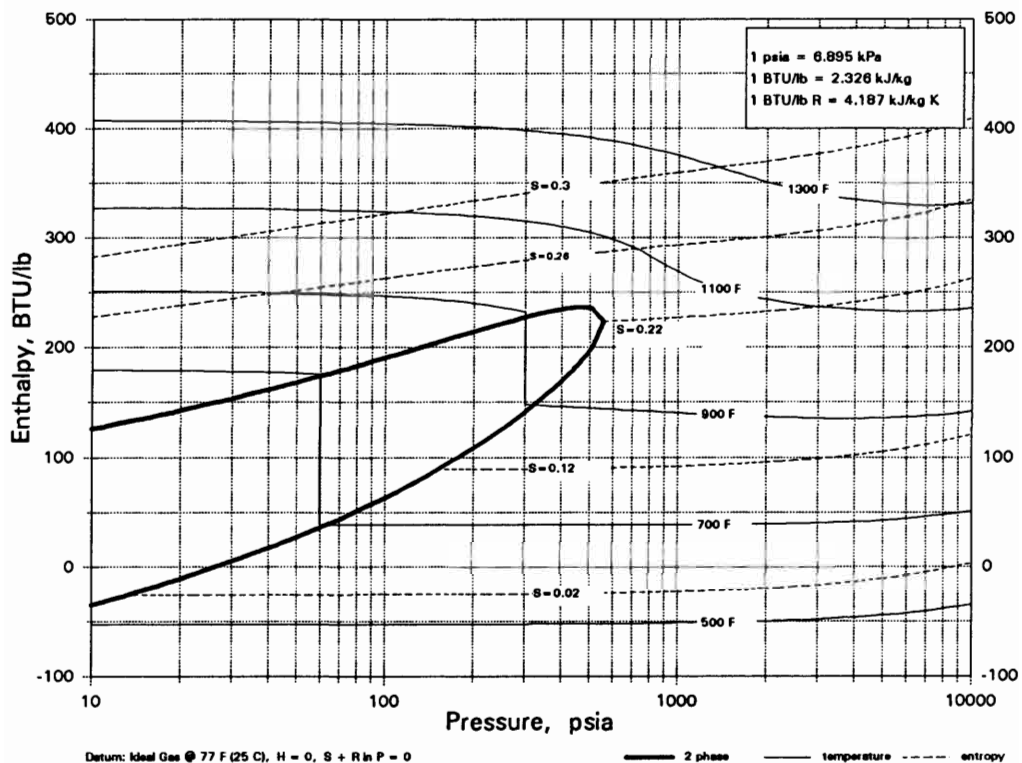
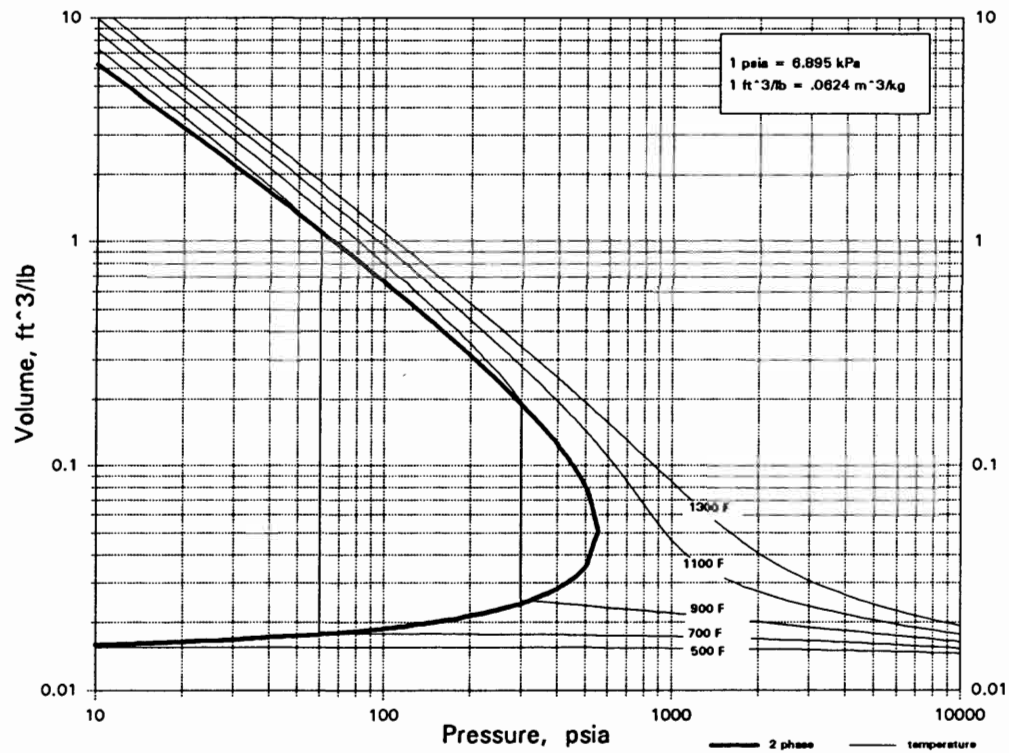
C6H4N2O4

o-DINITROBENZENE



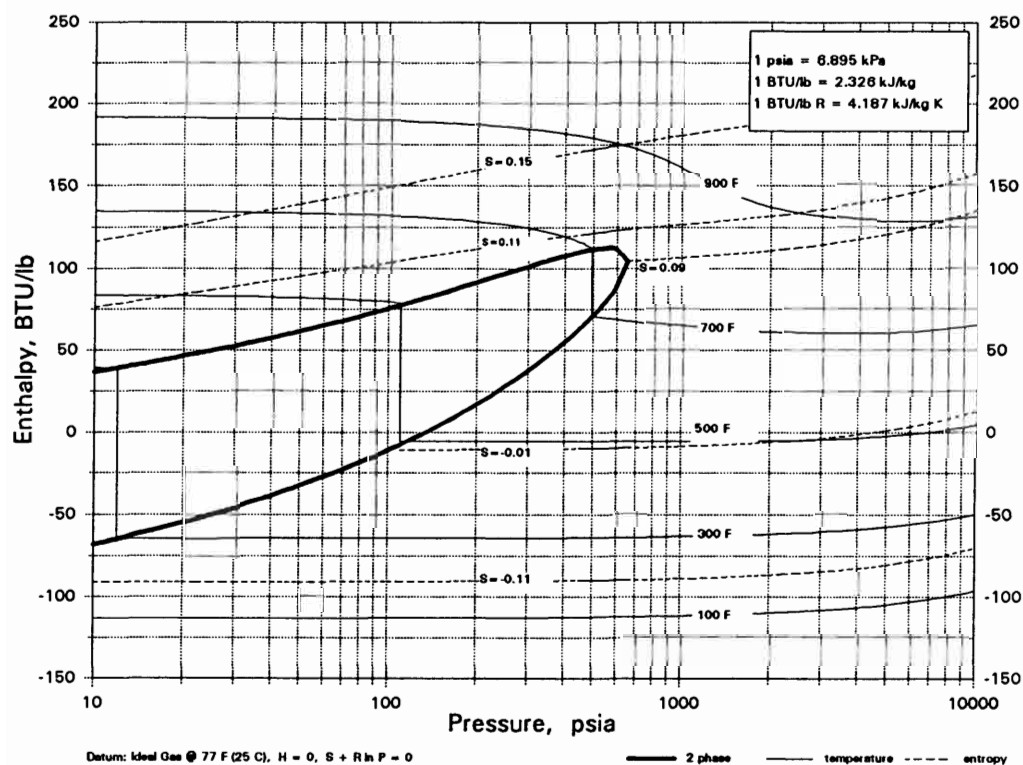
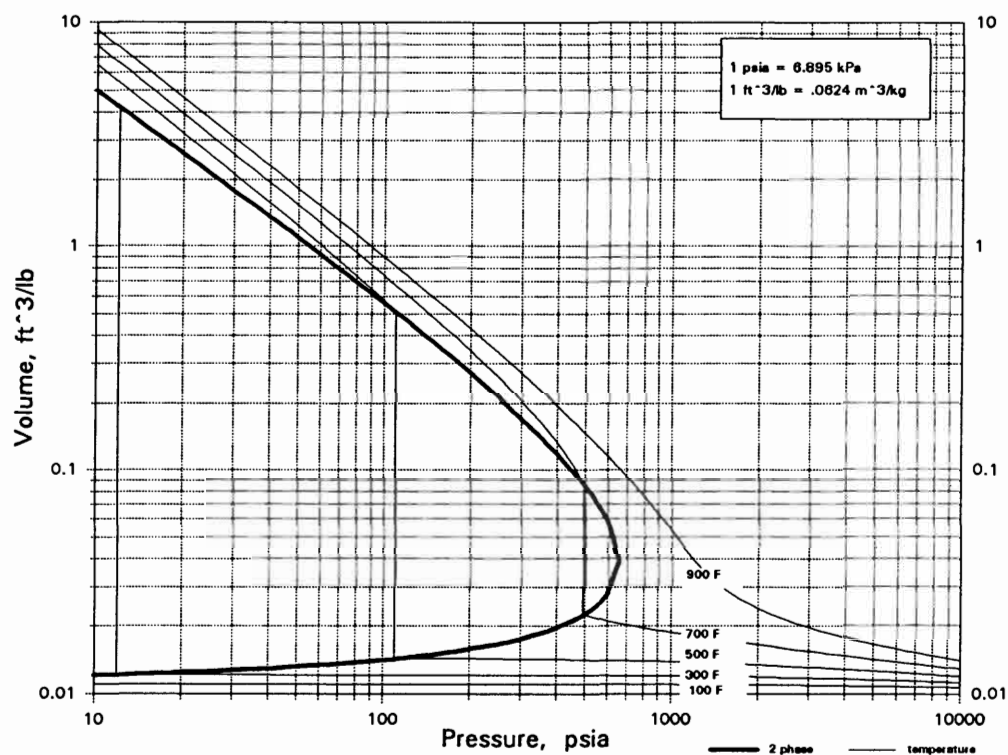
C6H4N2O4

p-DINITROBENZENE



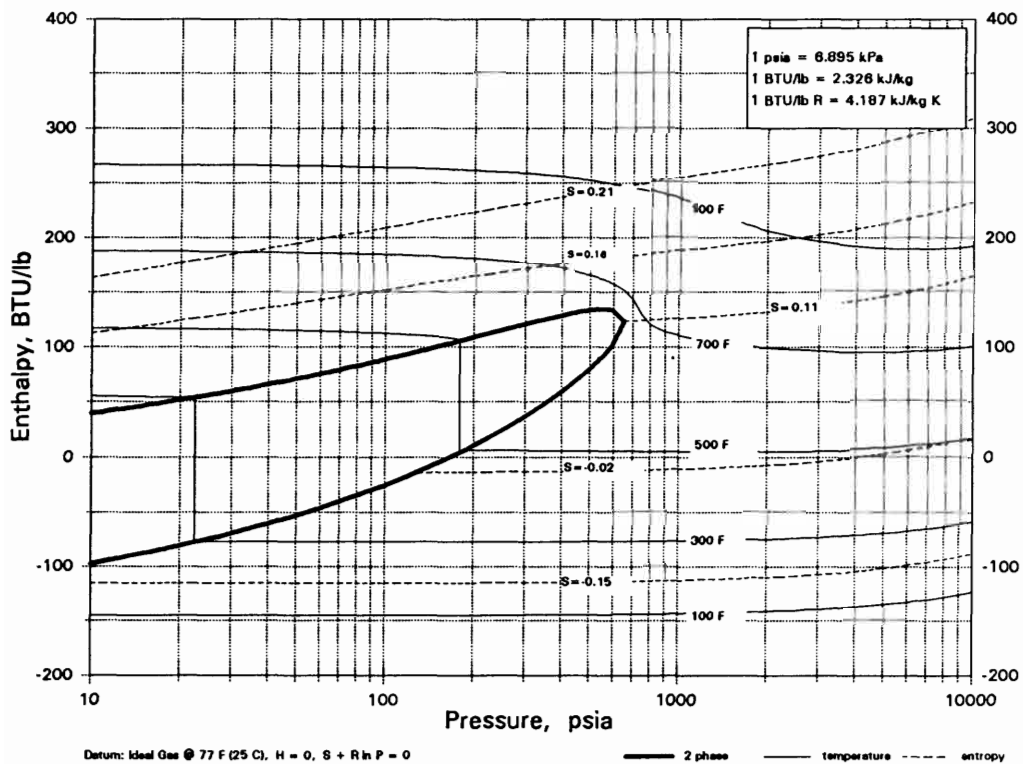
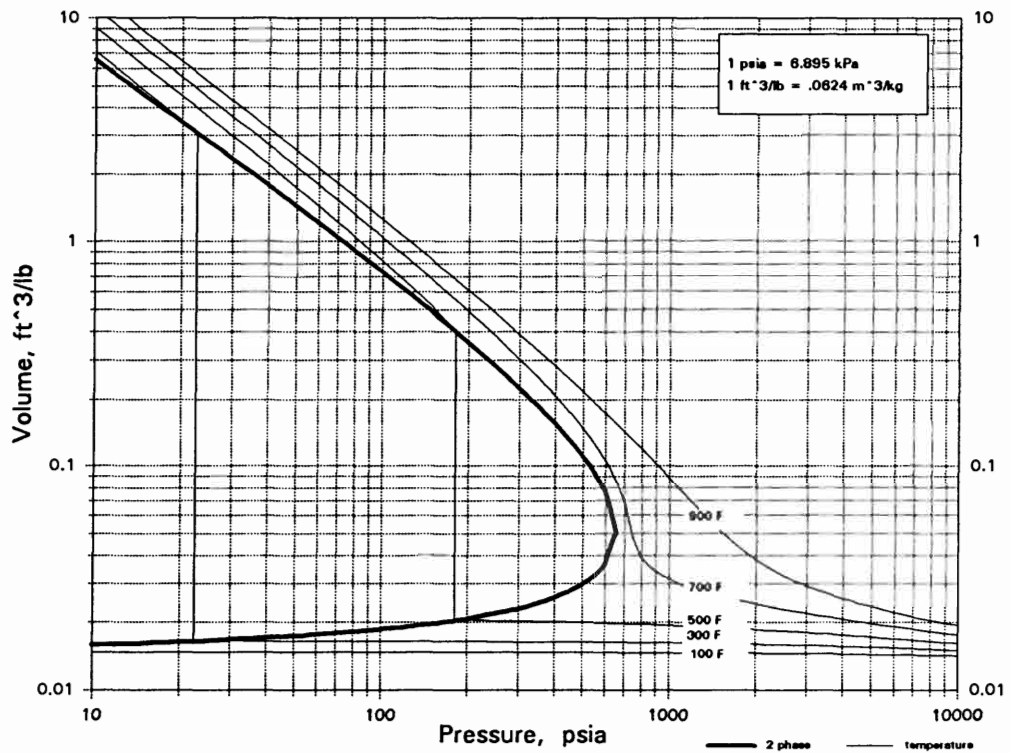
C6H5Br

BROMOBENZENE



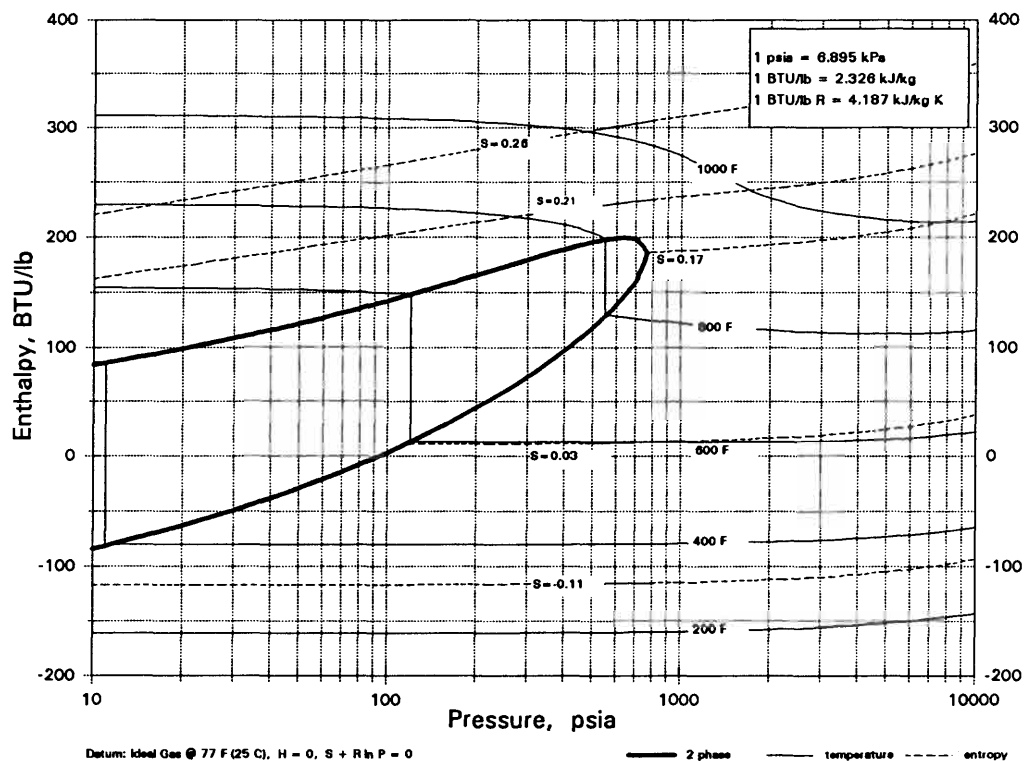
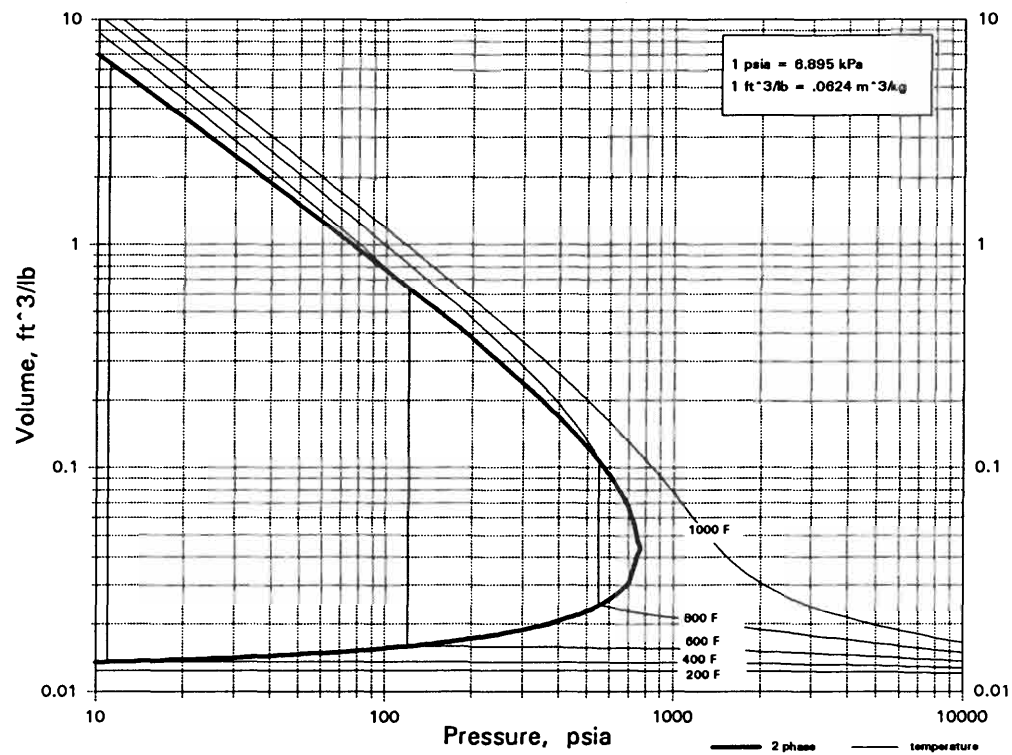
C6H5Cl

MONOCHLOROBENZENE



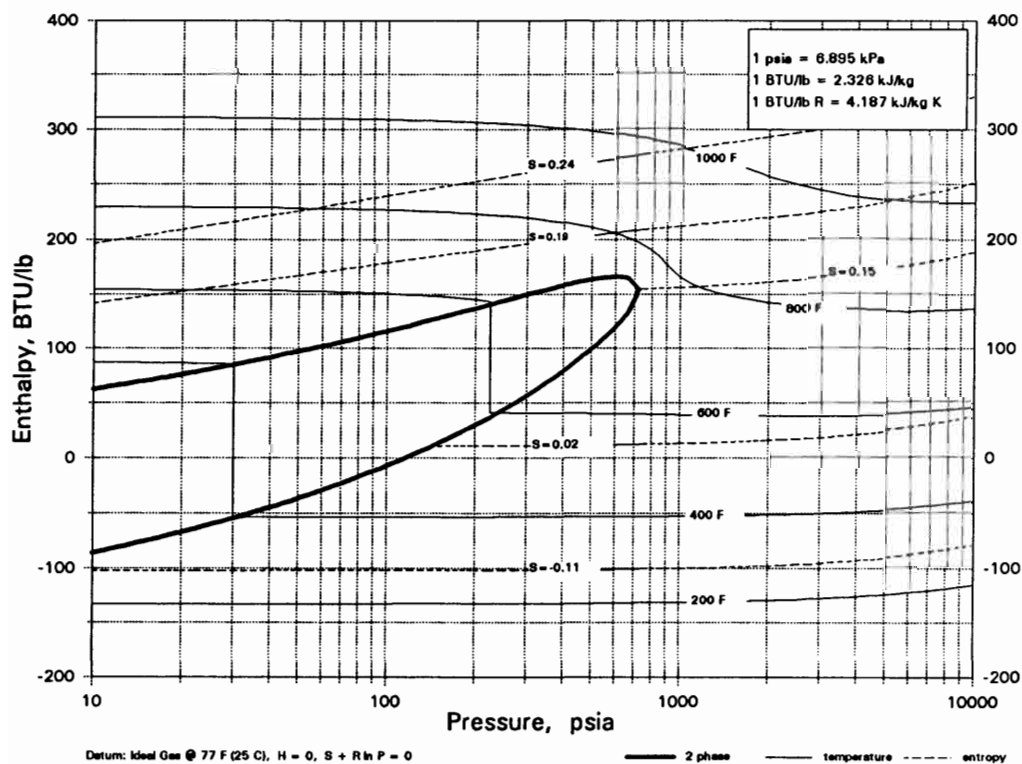
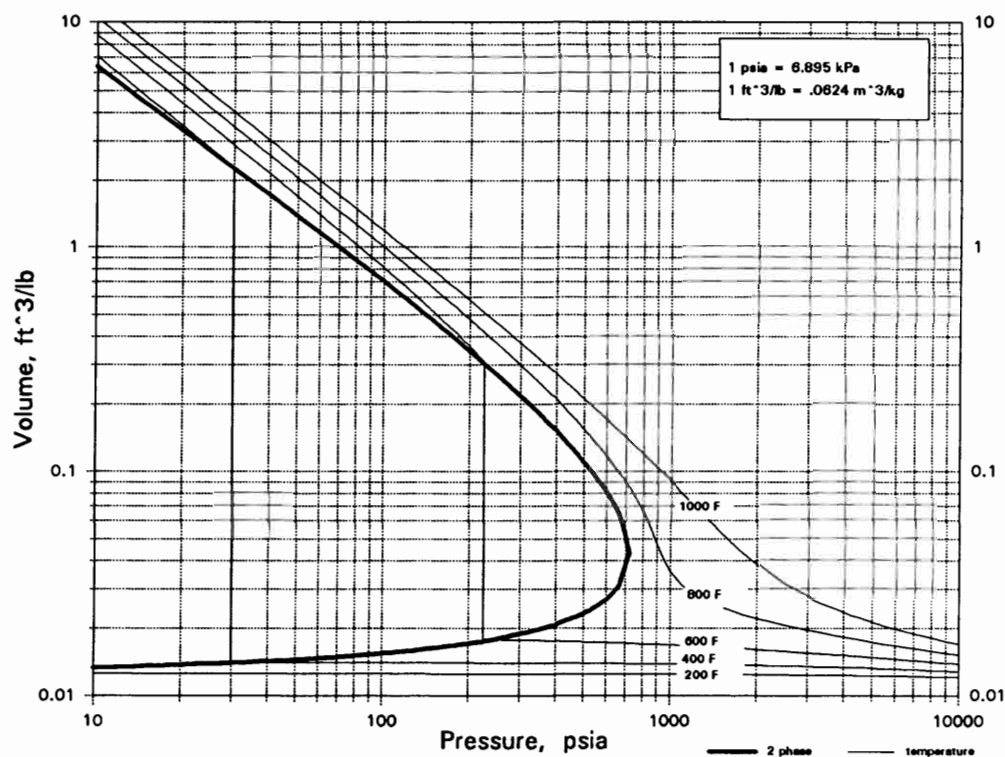
C6H5ClO

m-CHLOROPHENOL

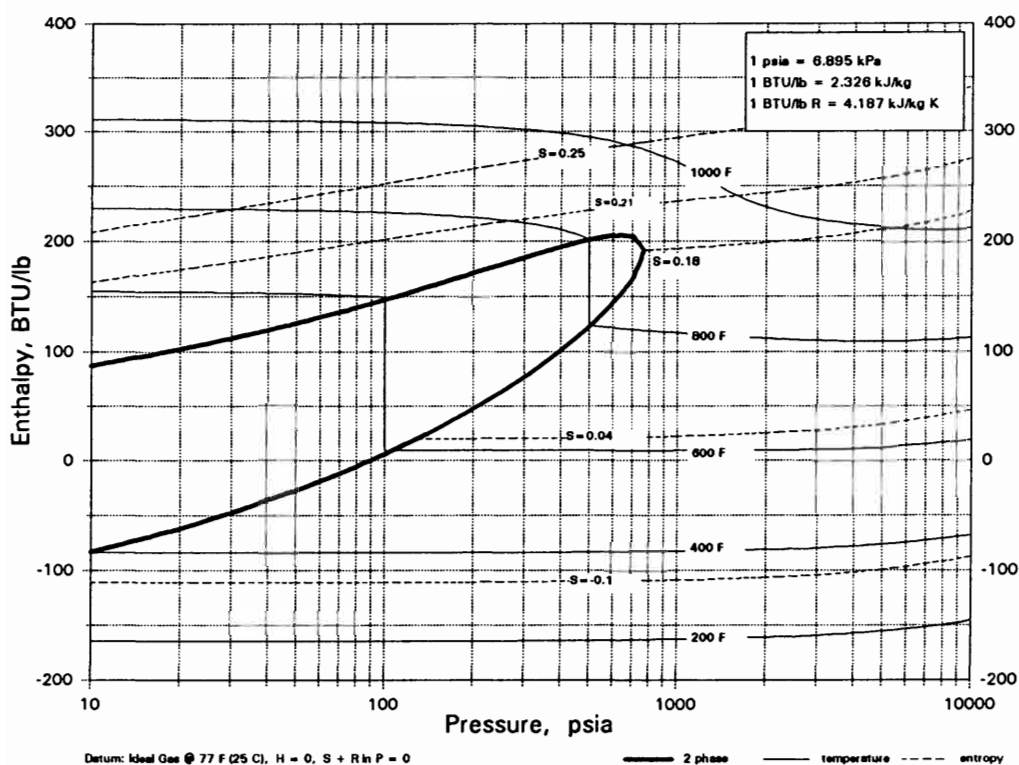
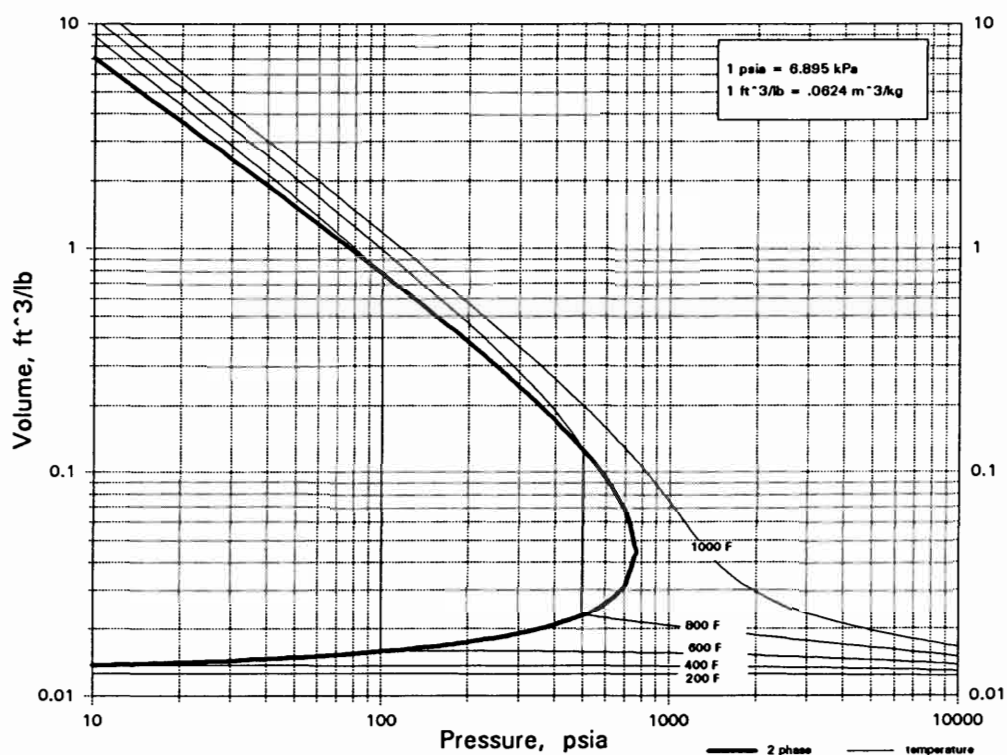


C₆H₅ClO

o-CHLOROPHENOL

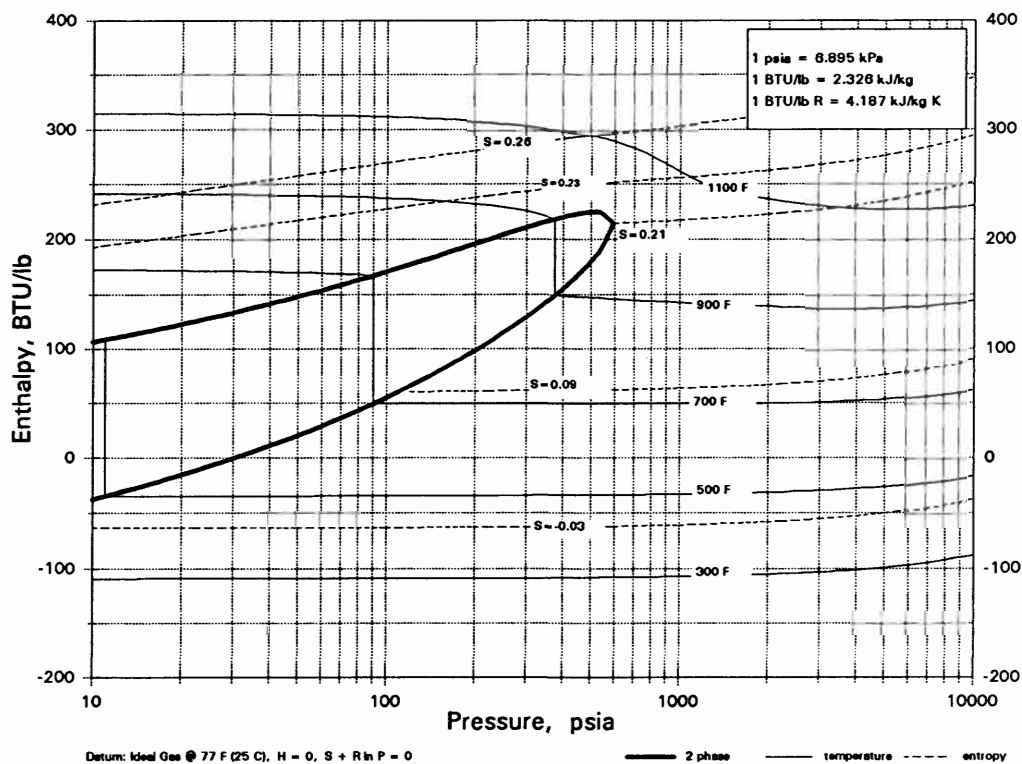
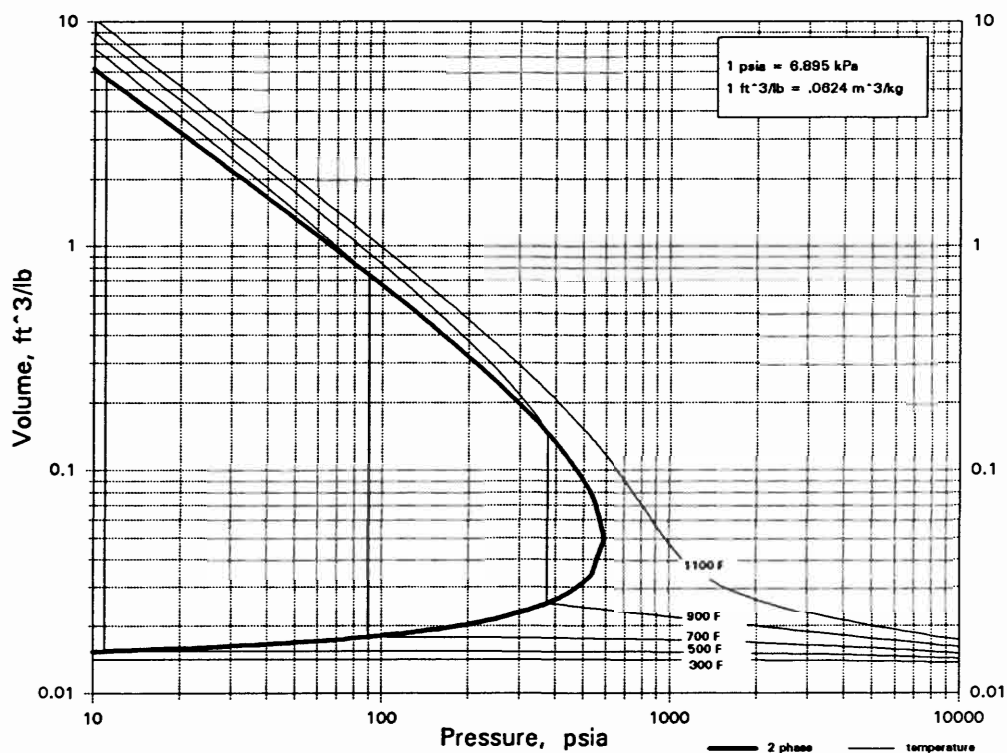


C₆H₅ClO p-CHLOROPHENOL



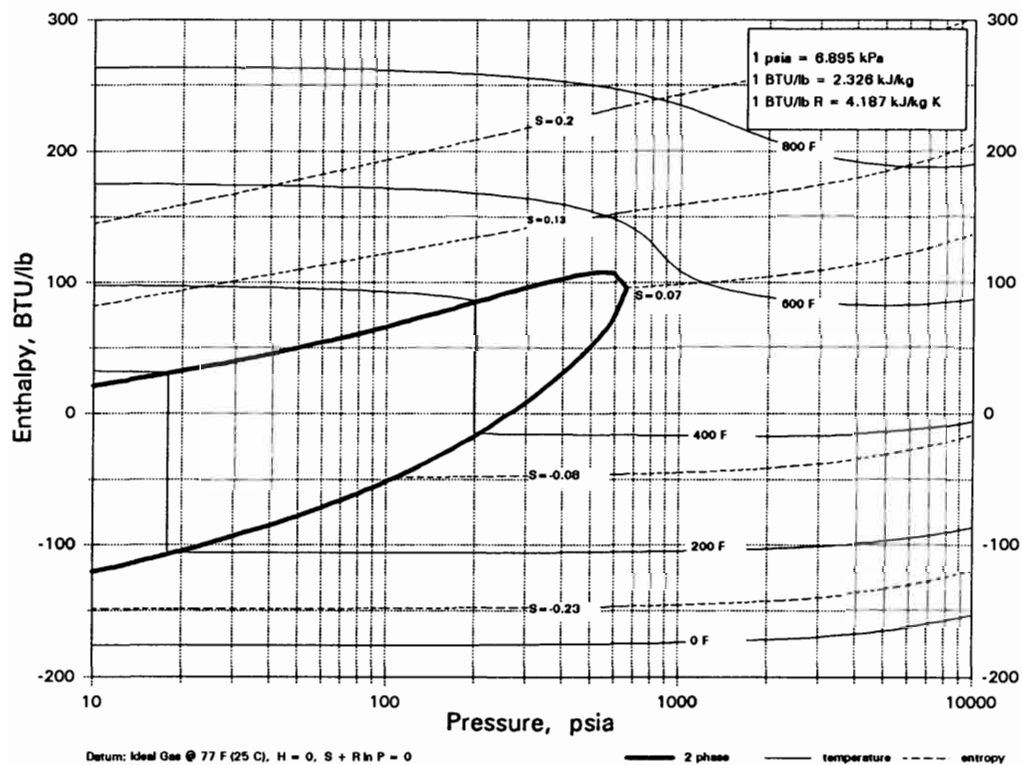
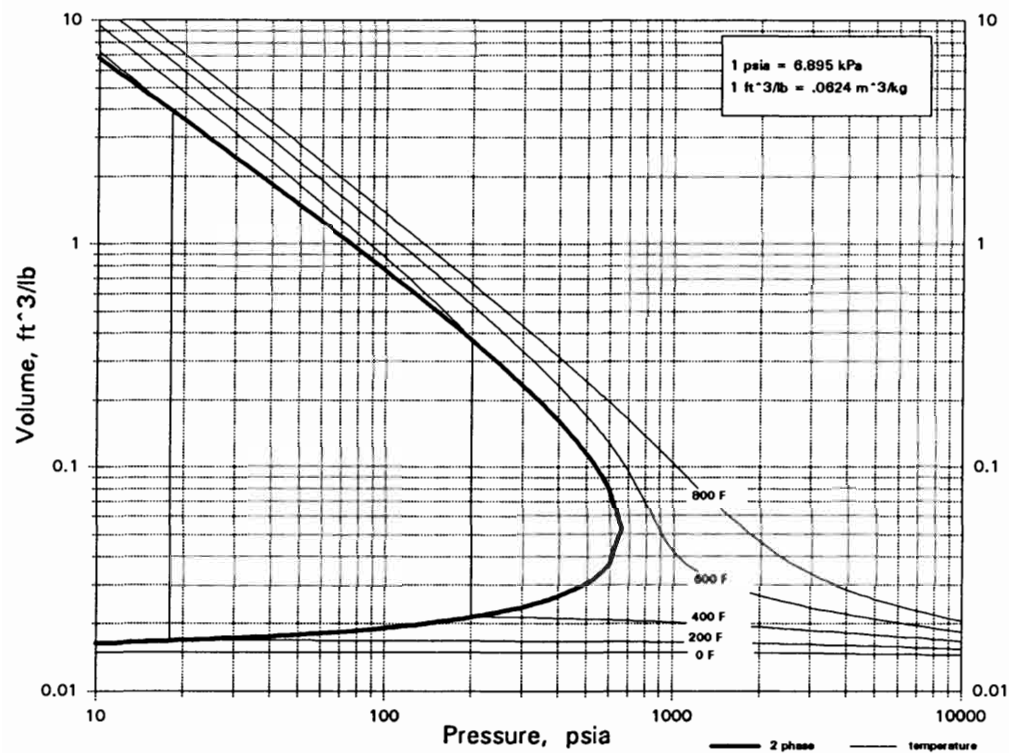
C6H5Cl2N

3-4-DICHLOROANILINE

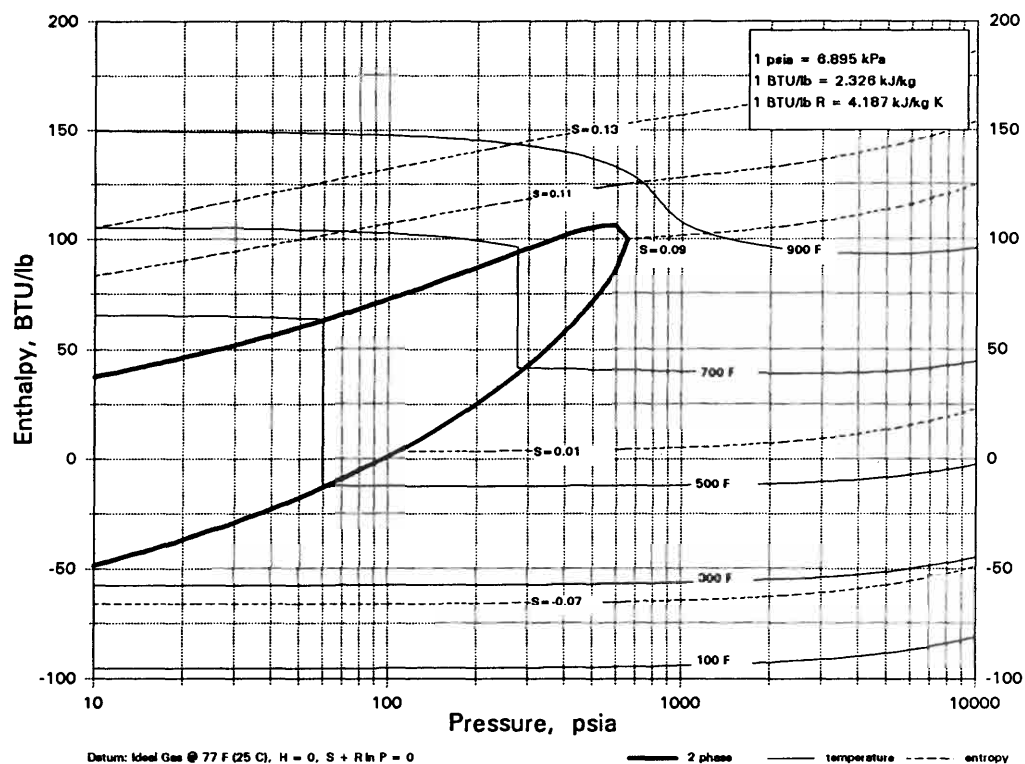
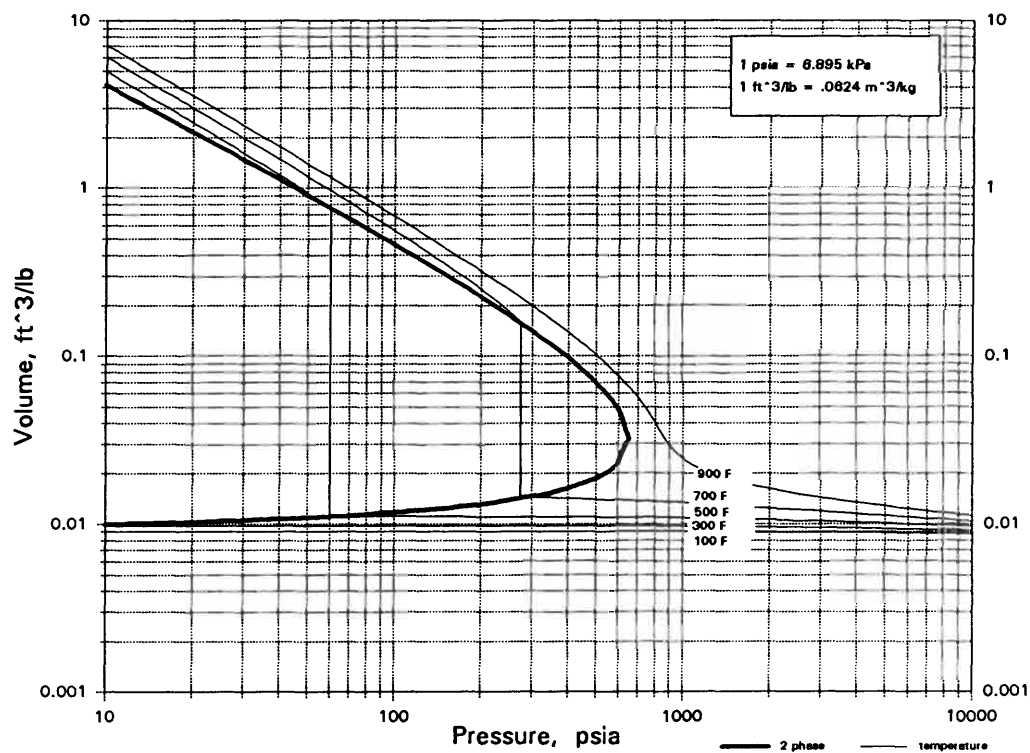


C6H5F

FLUOROBENZENE

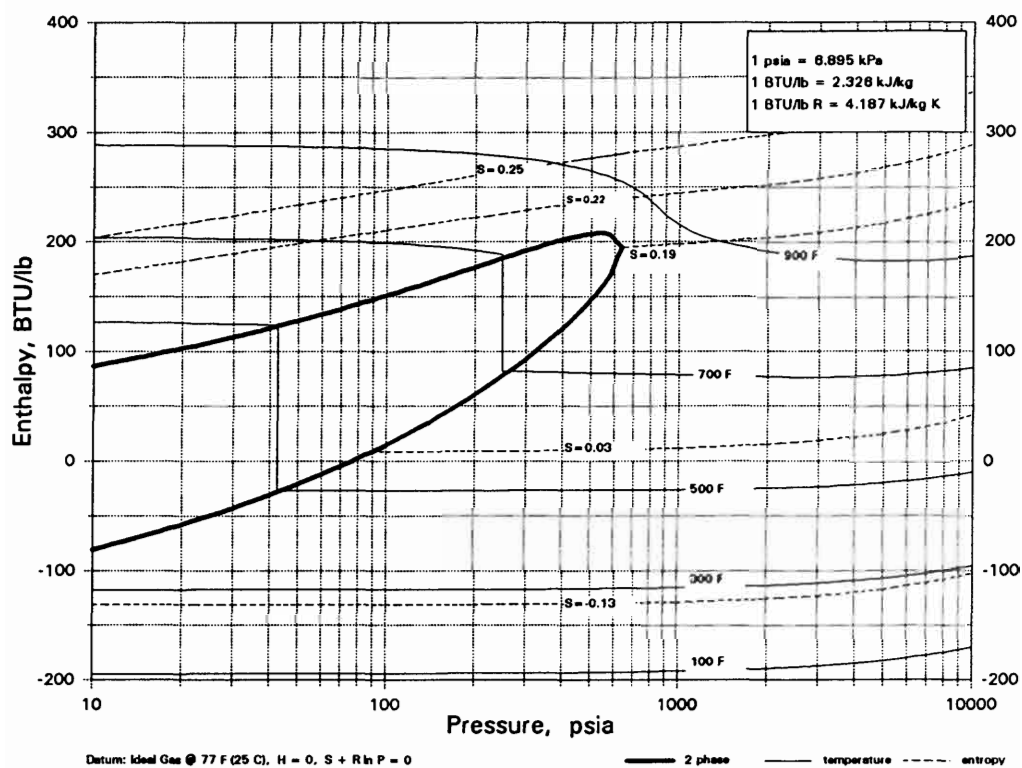
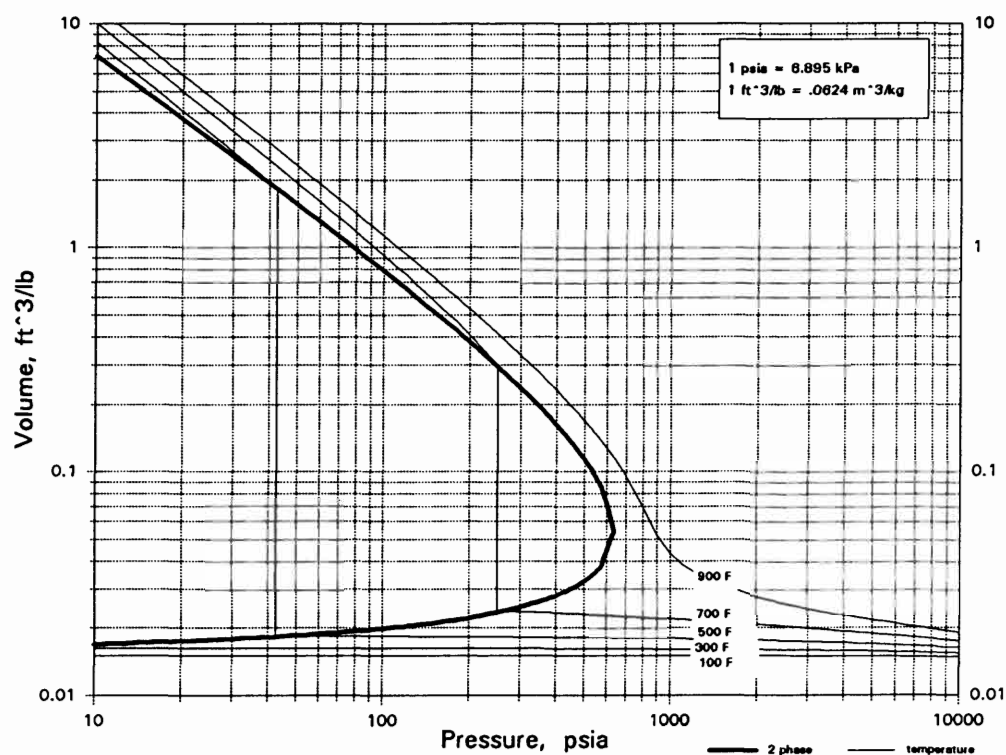


C6H5I
IODOBENZENE



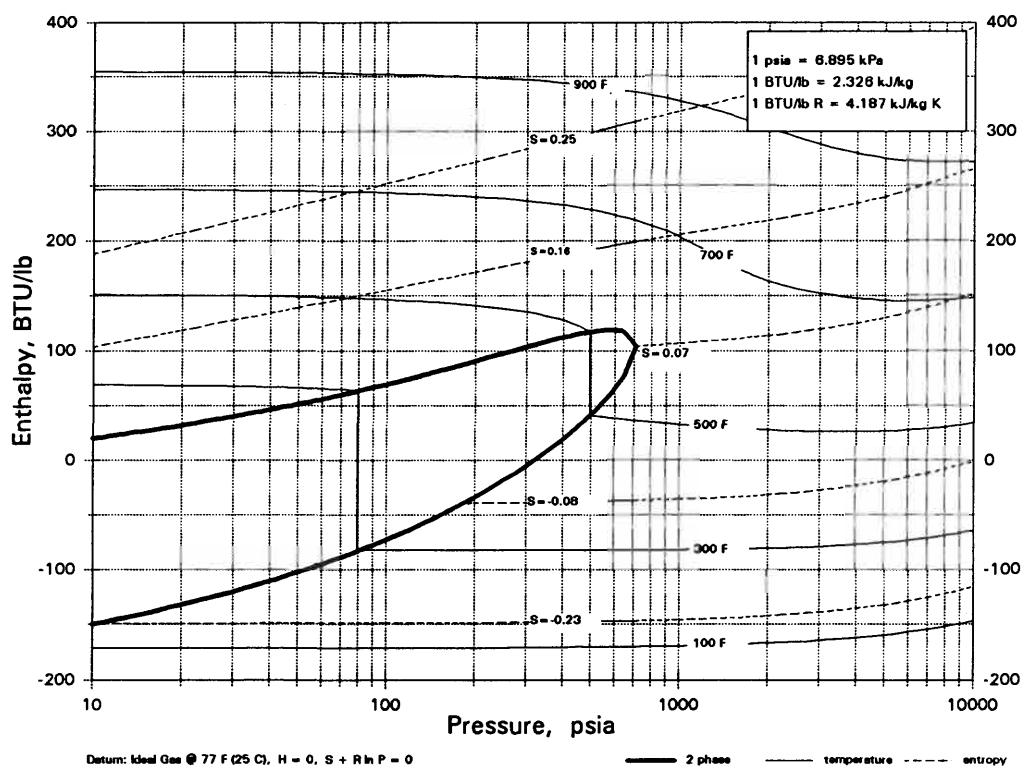
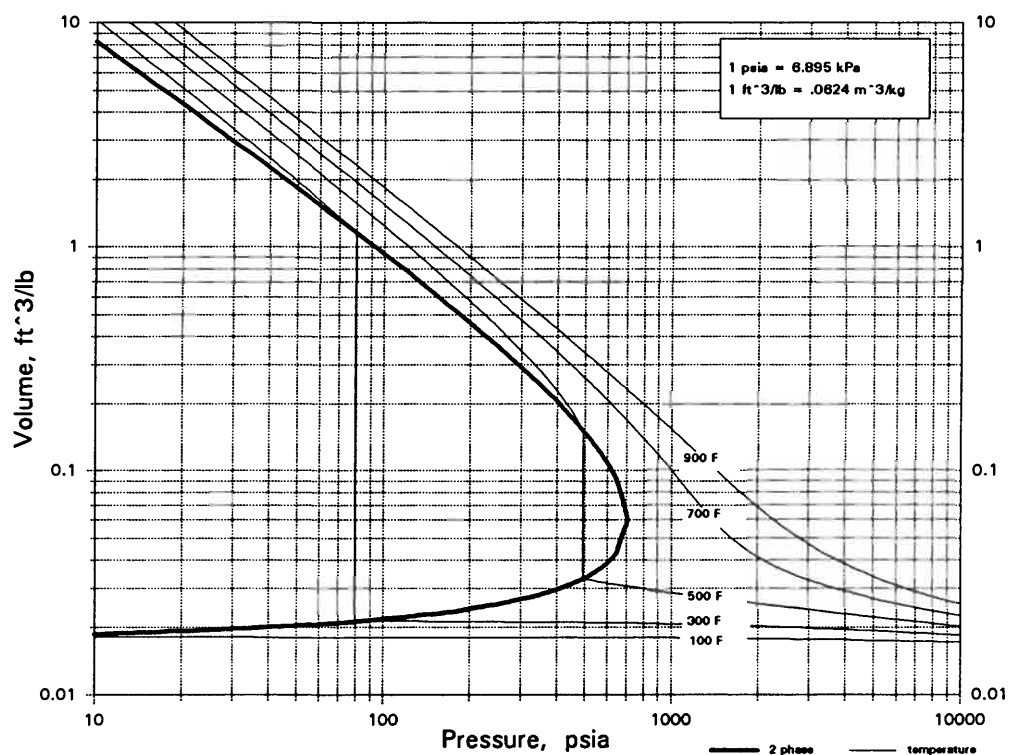
C6H5NO2

NITROBENZENE



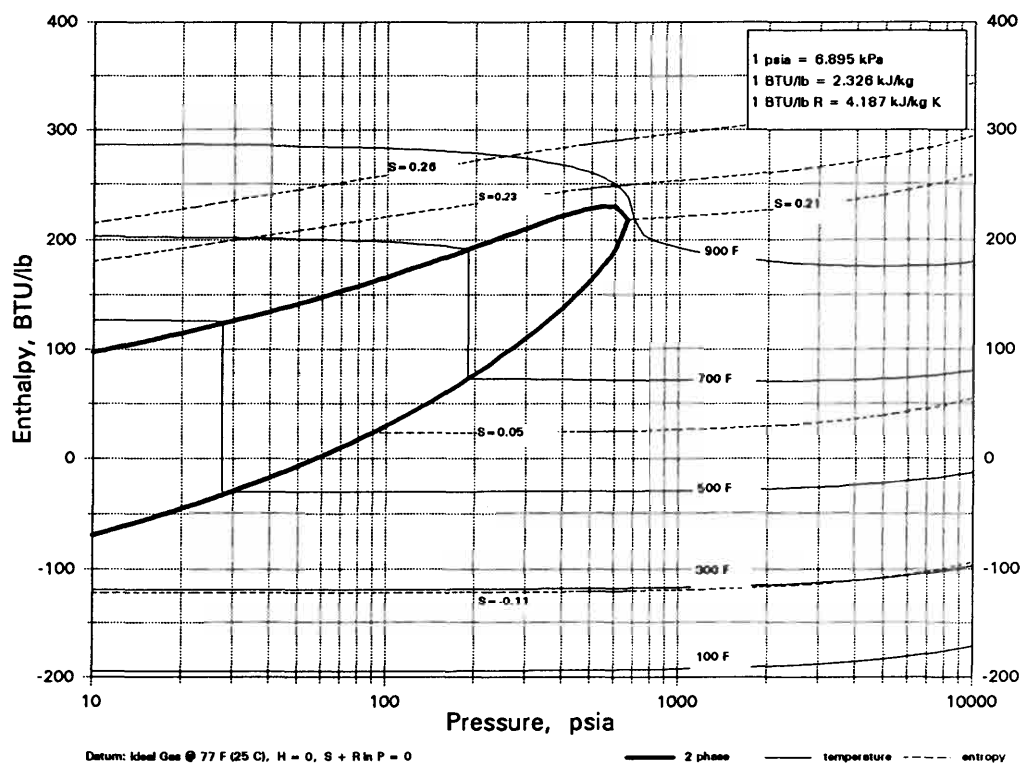
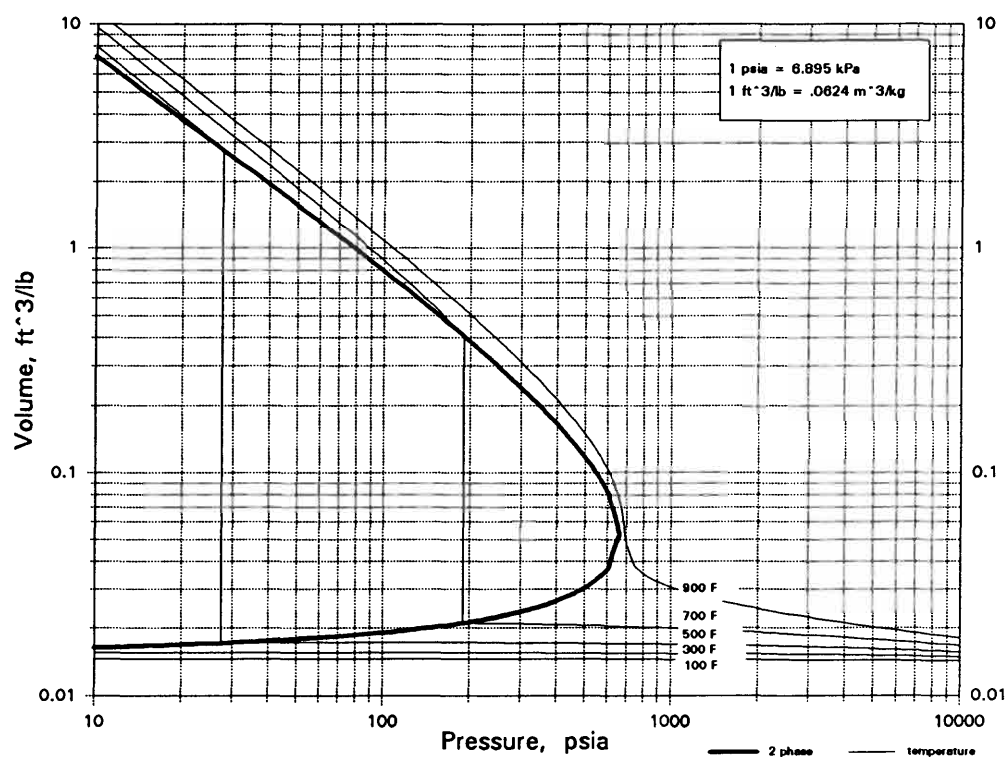
C6H6

BENZENE



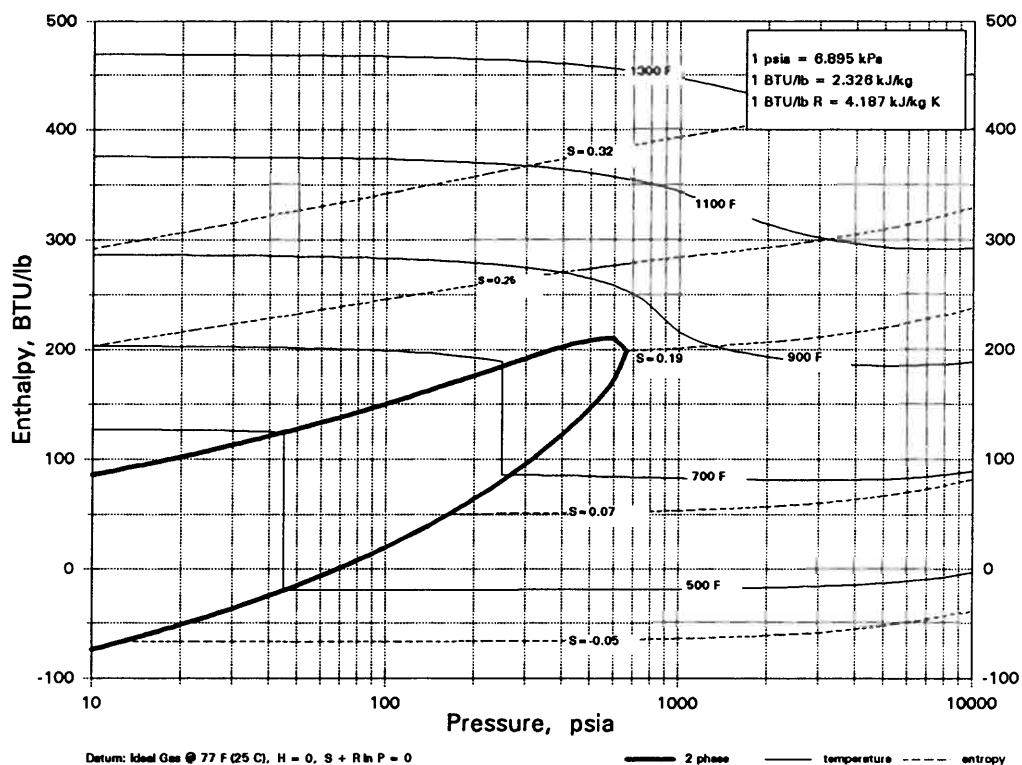
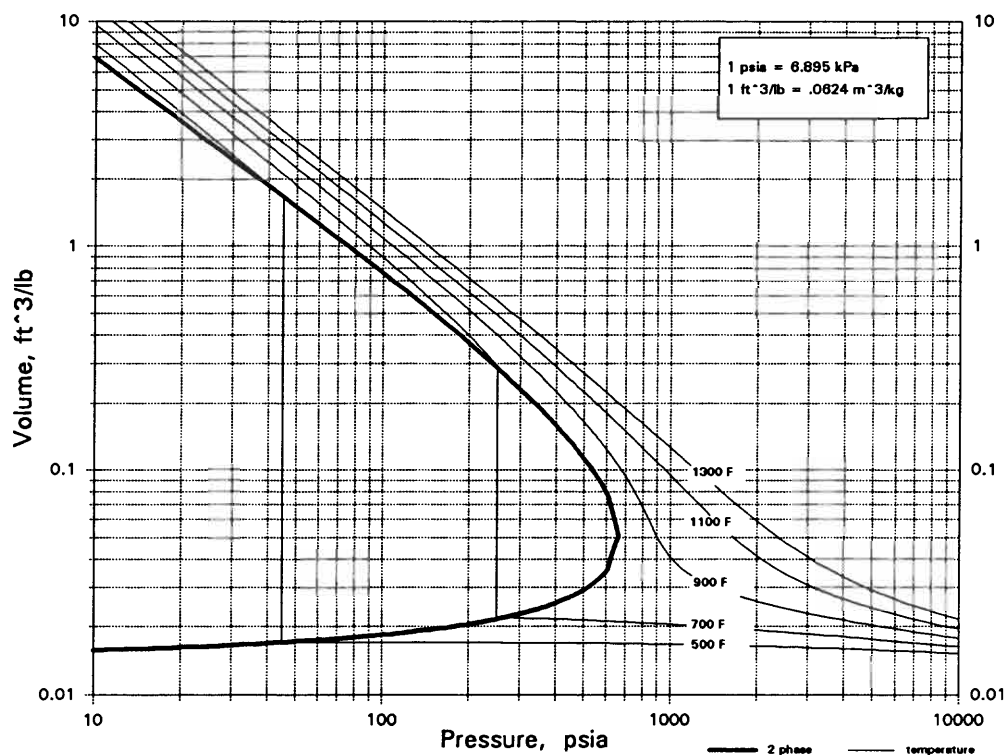
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m-CHLOROANILINE



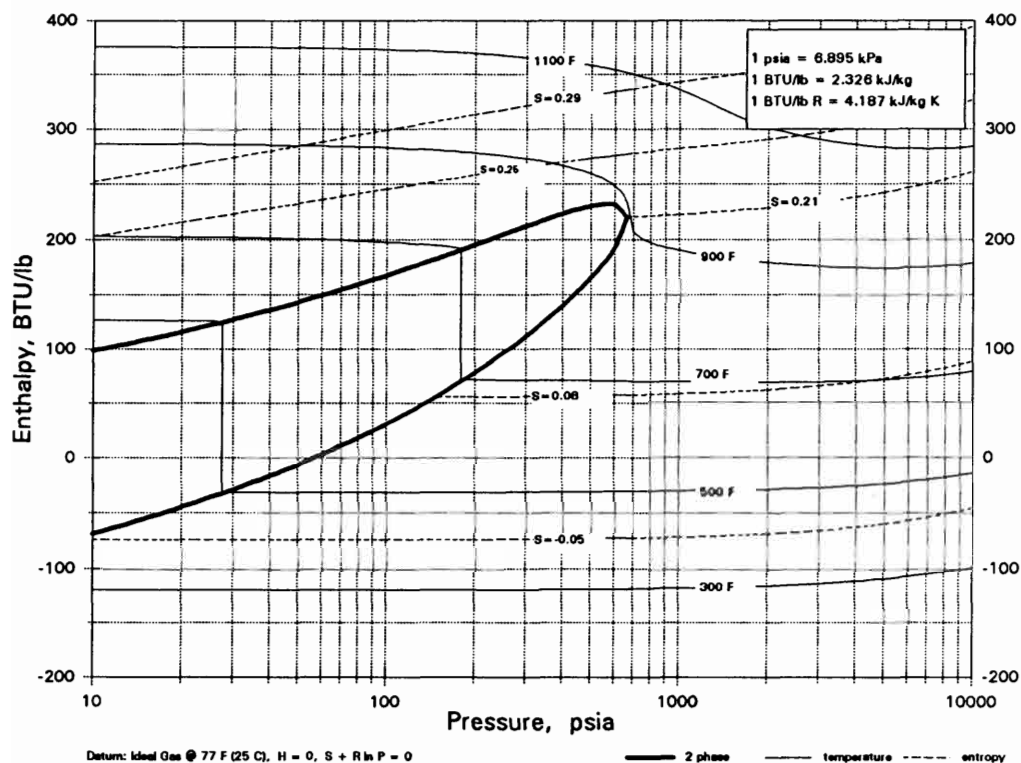
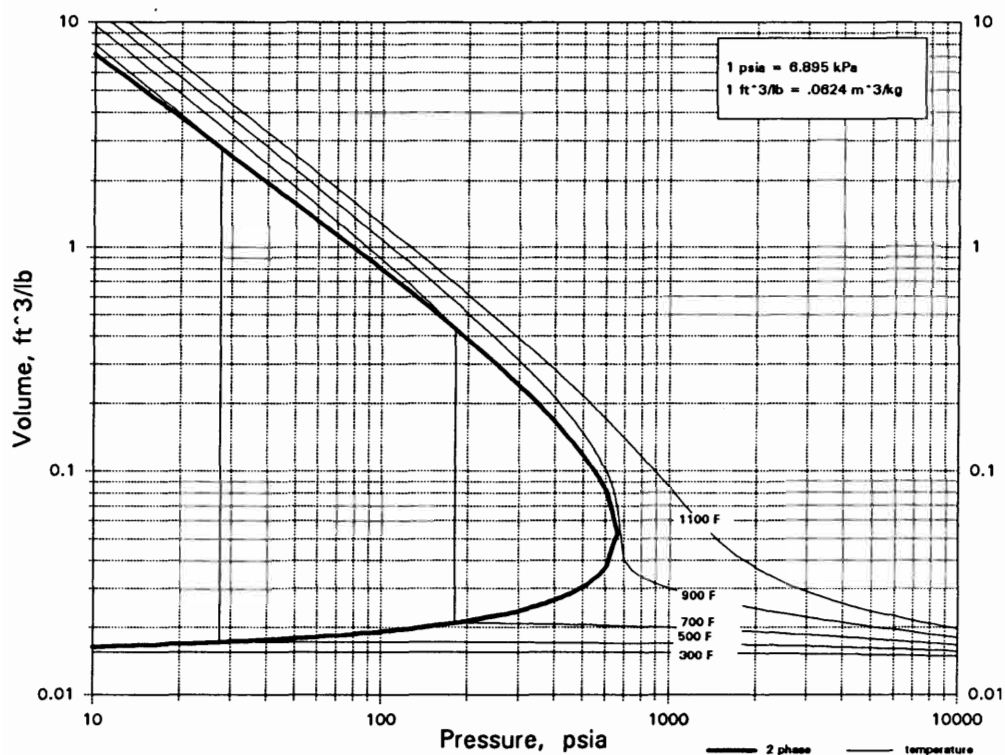
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o-CHLOROANILINE



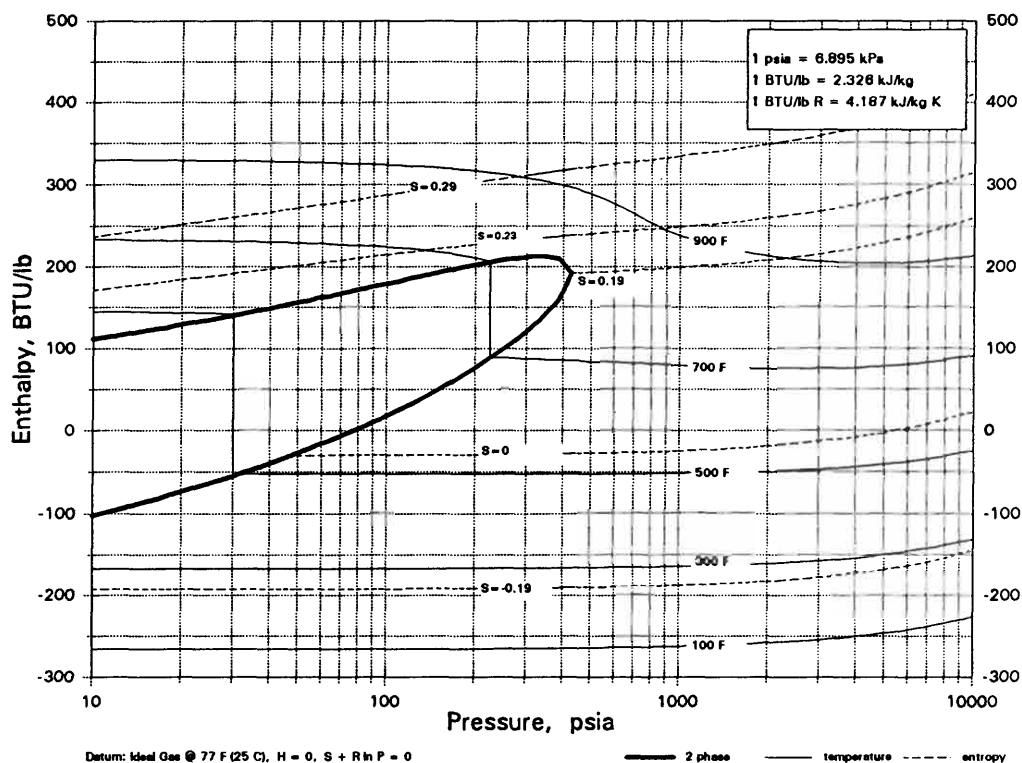
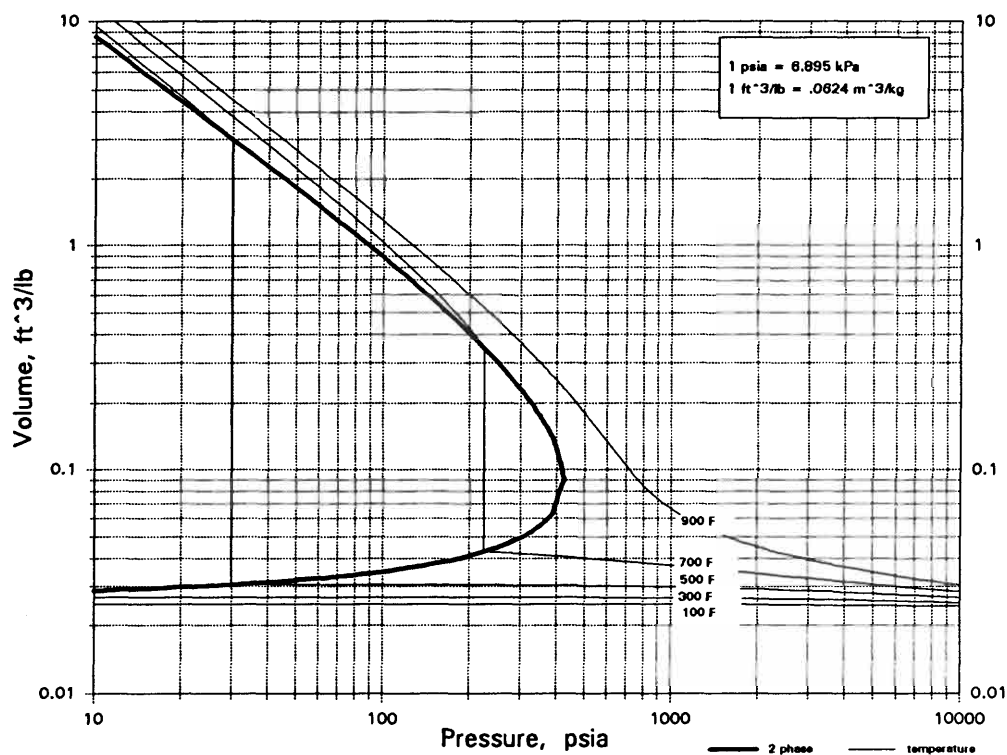
C6H6ClN

p-CHLOROANILINE



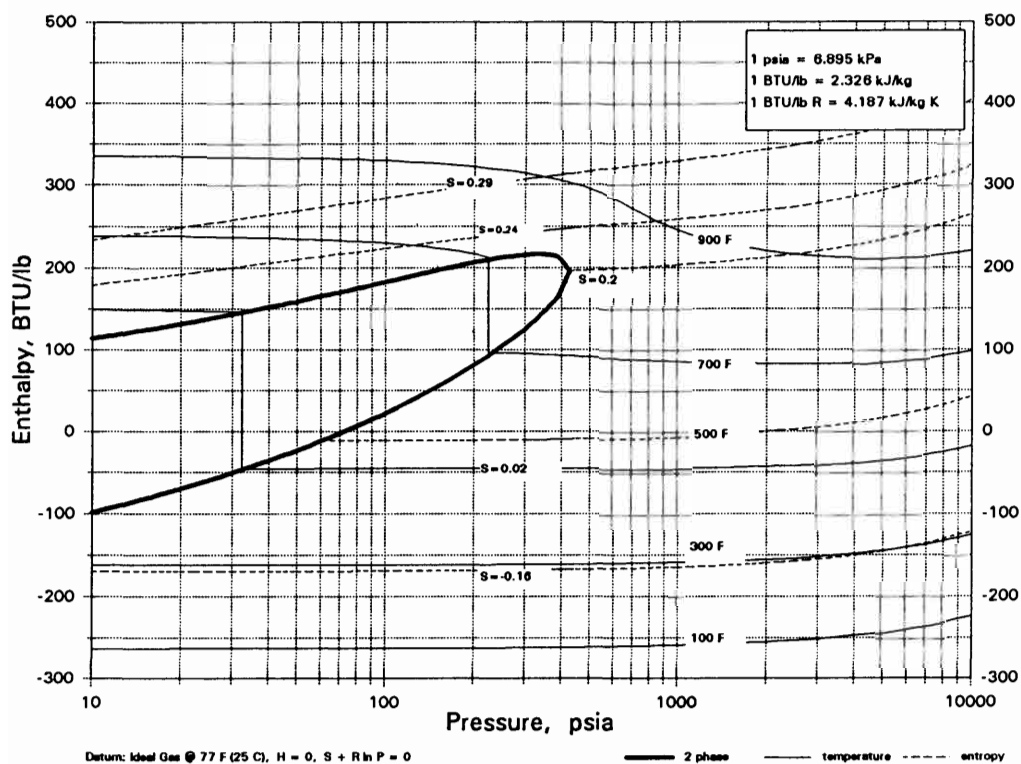
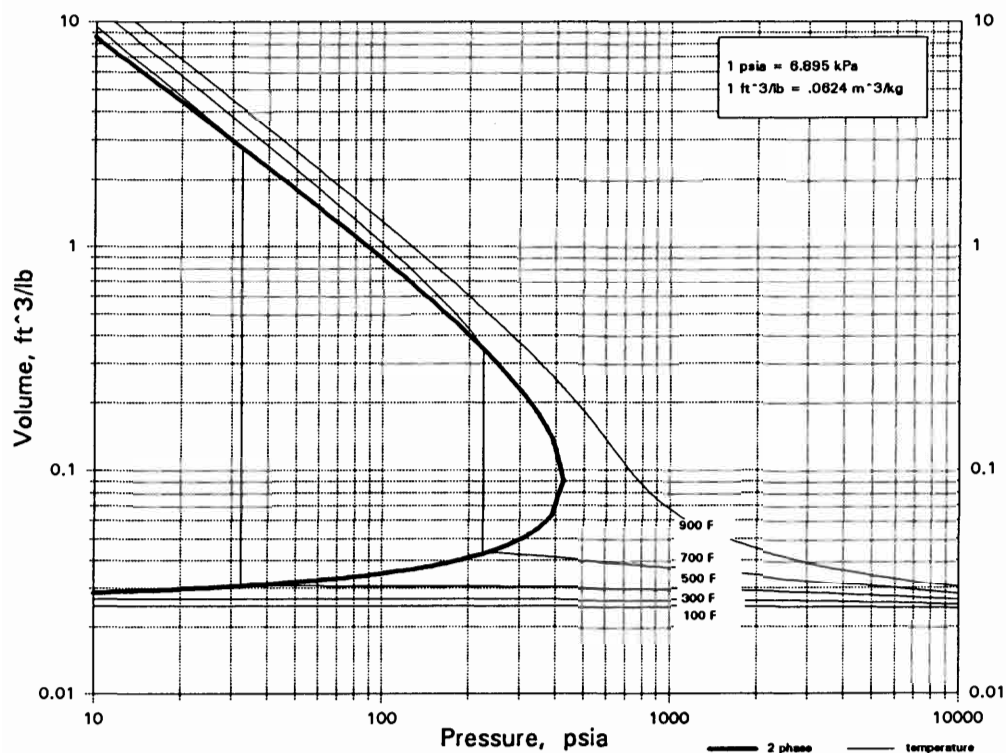
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cis-DICYANO-1-BUTENE



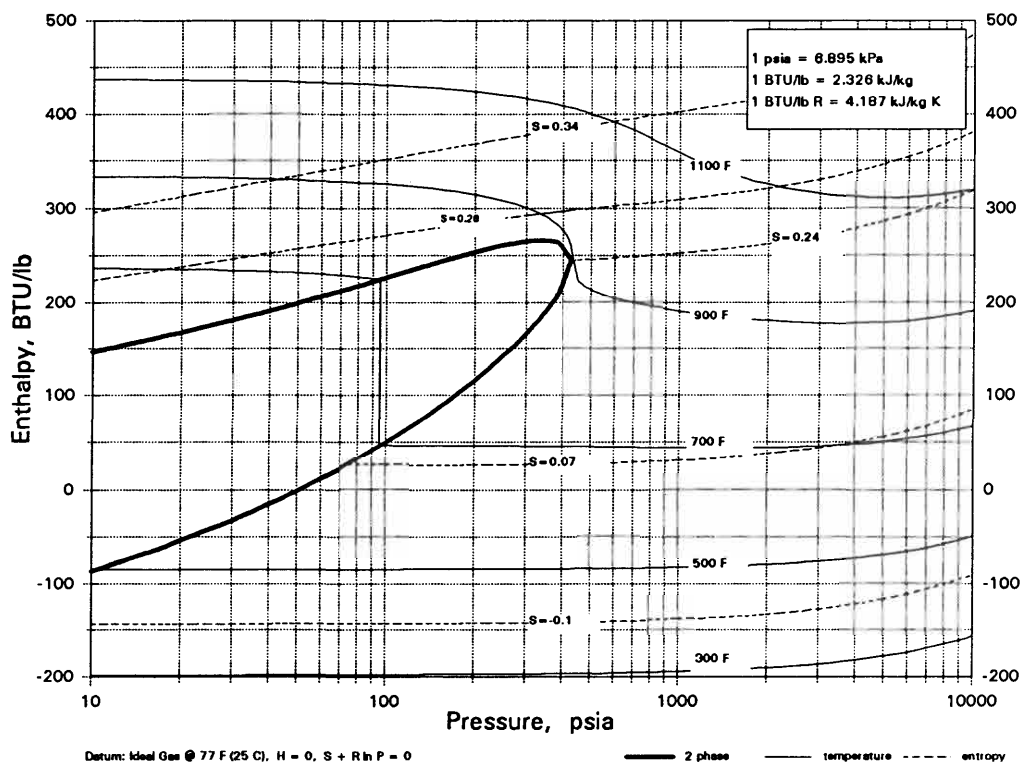
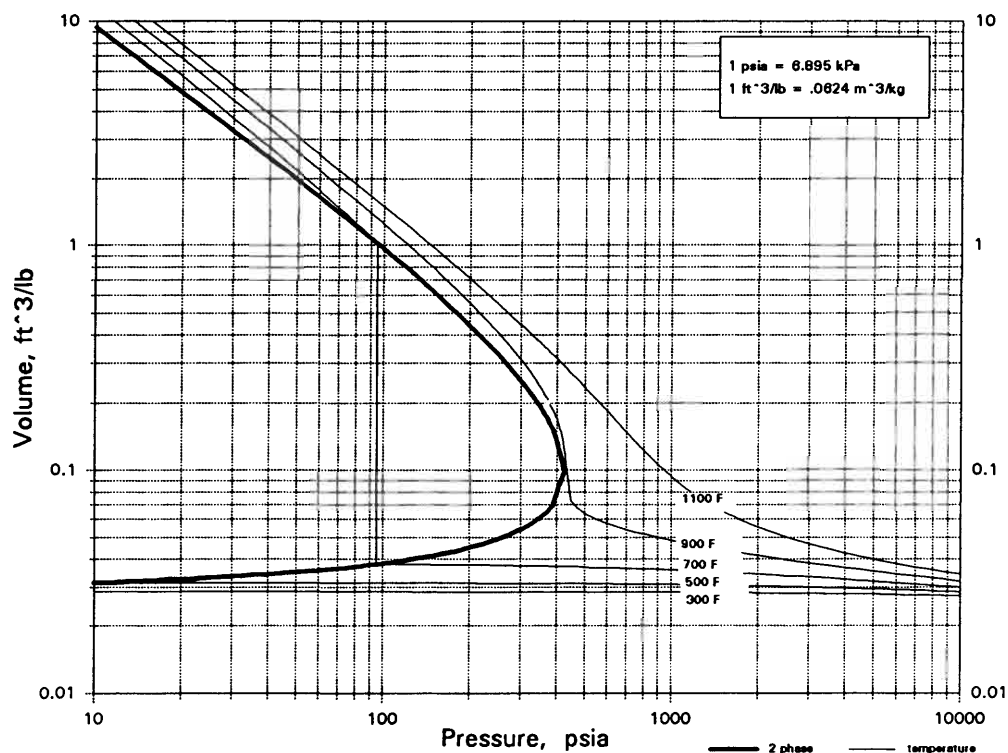
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trans-DICYANO-1-BUTENE

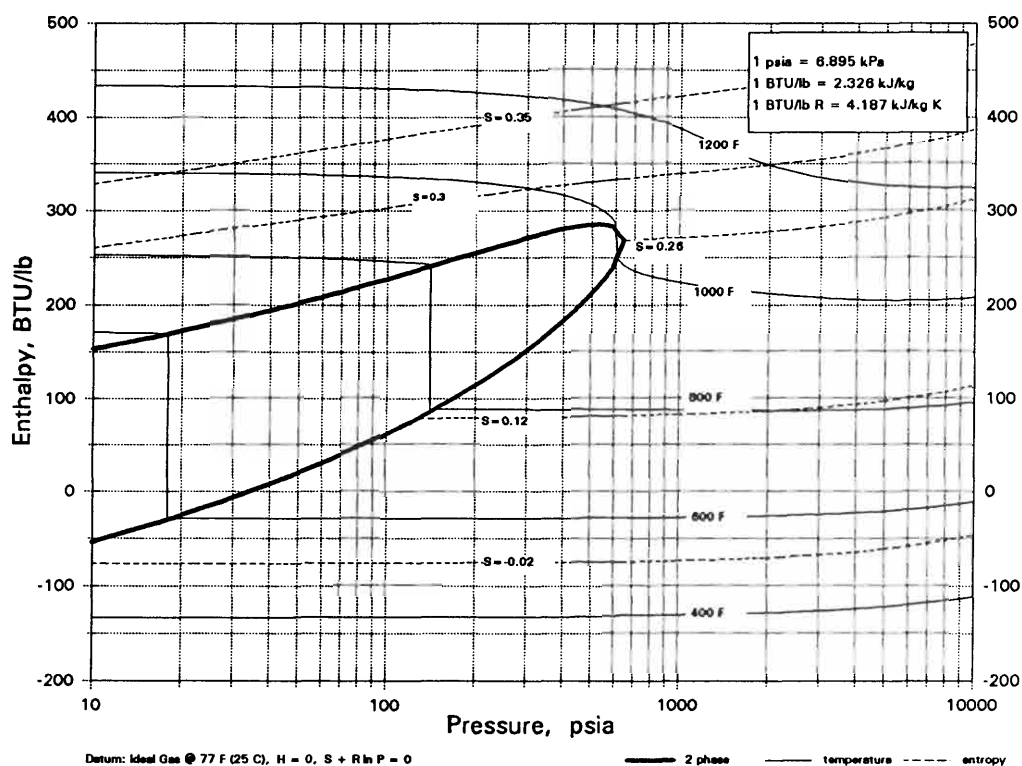
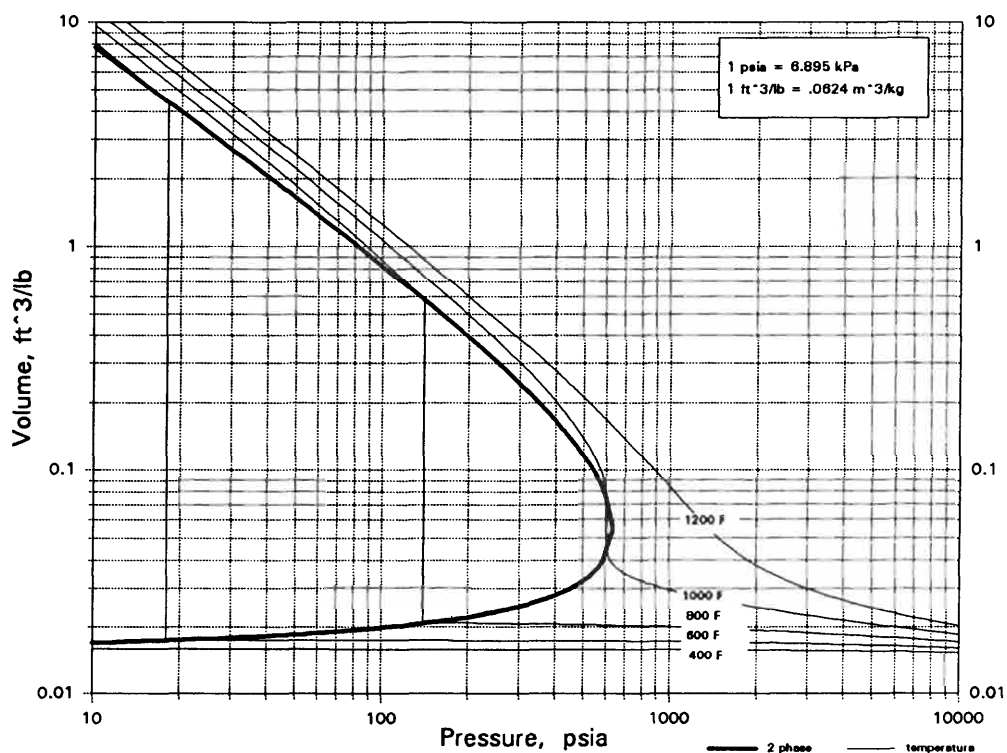


C6H6N2

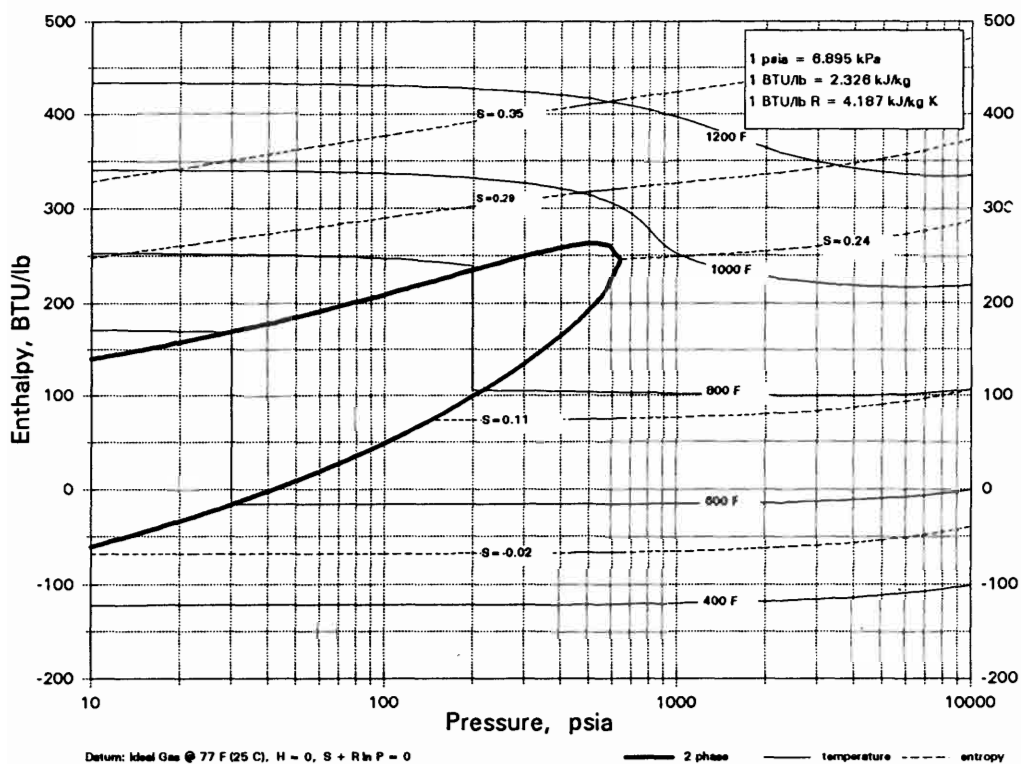
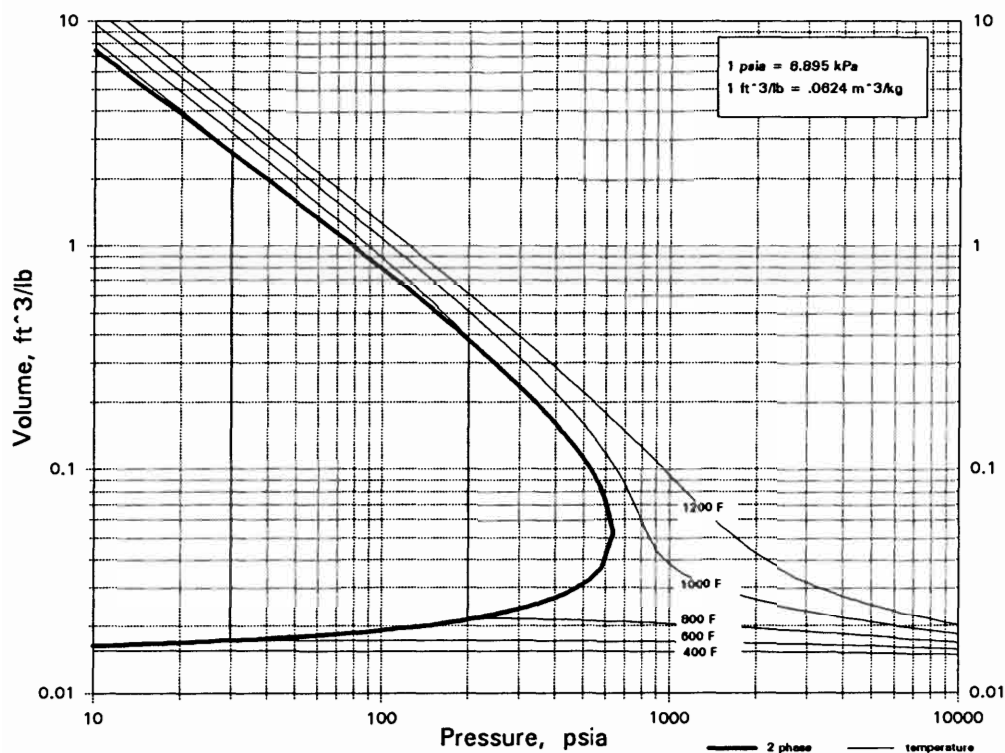
1-4-DICYANO-2-BUTENE



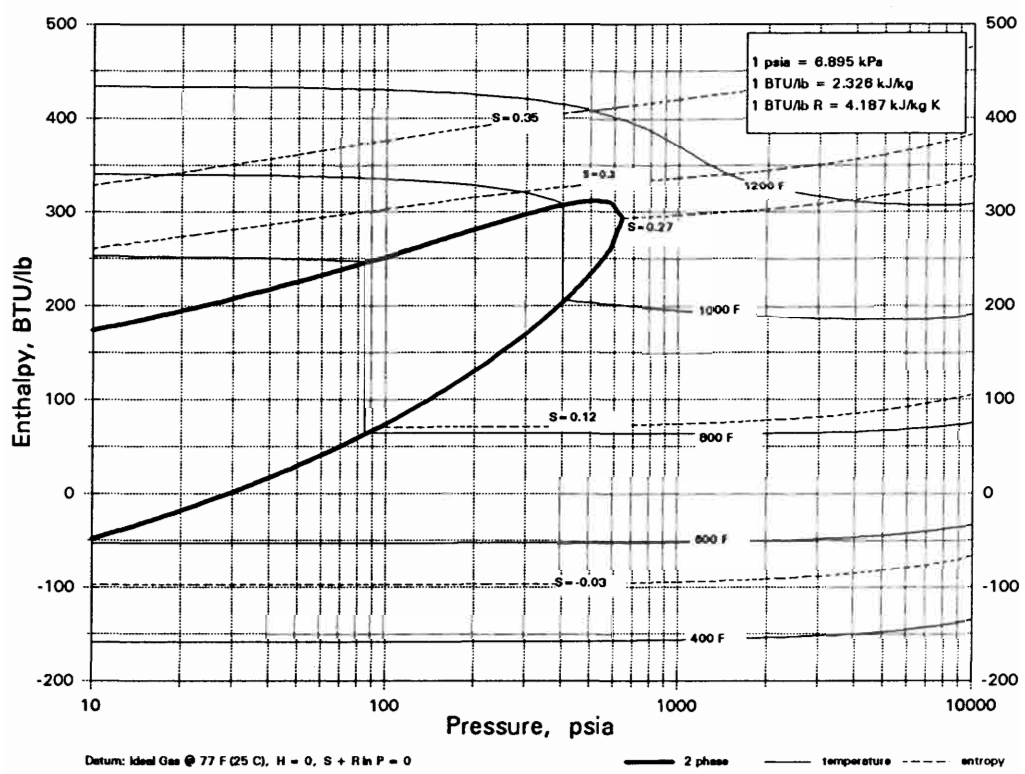
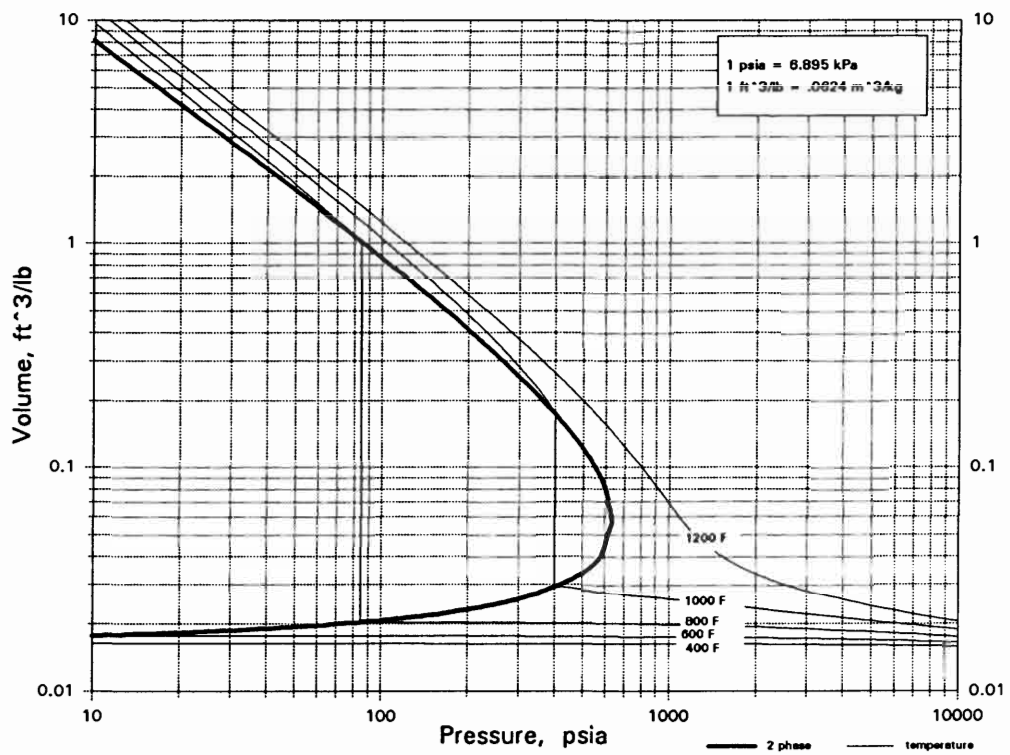
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C6H6N2O2 o-NITROANILINE

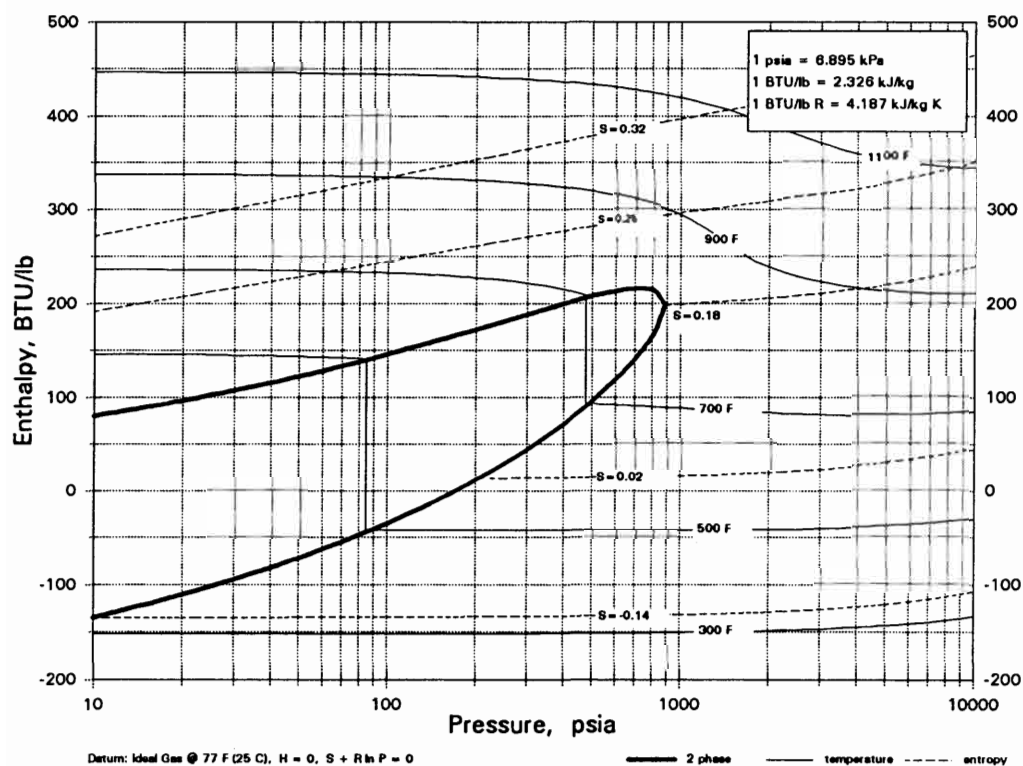
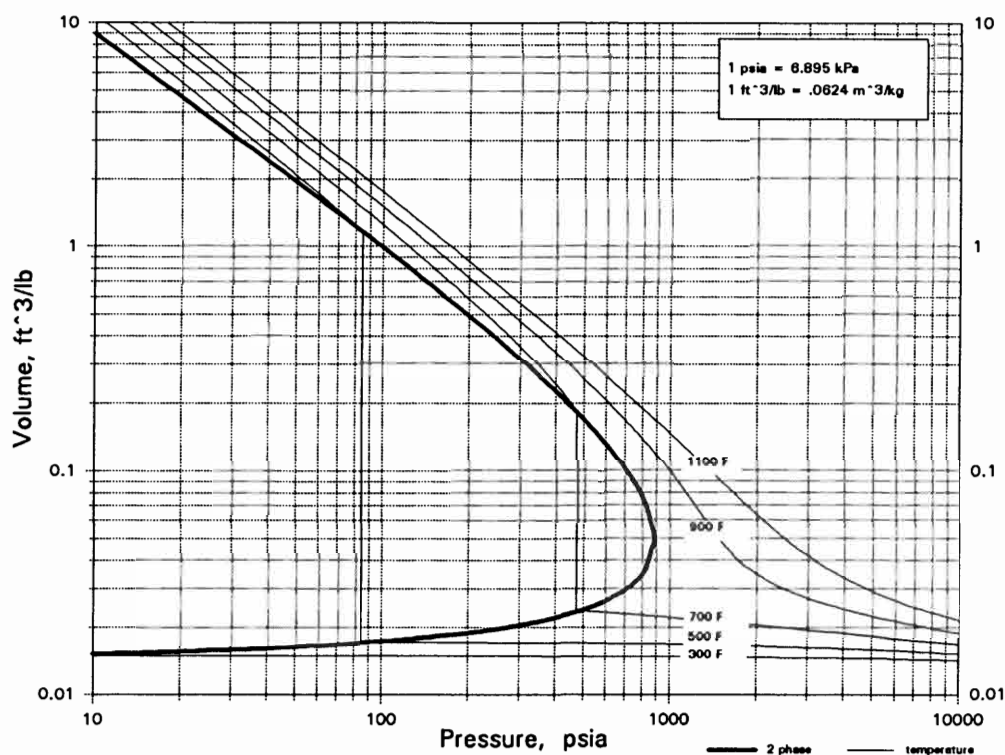


C6H6N2O2
p-NITROANILINE



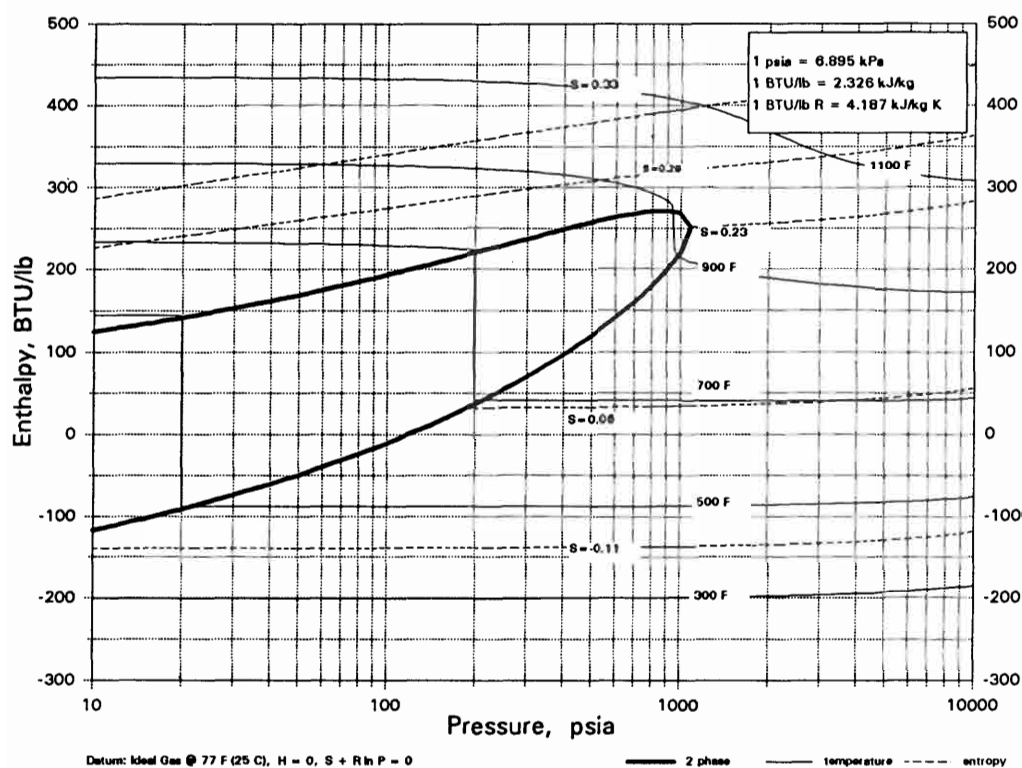
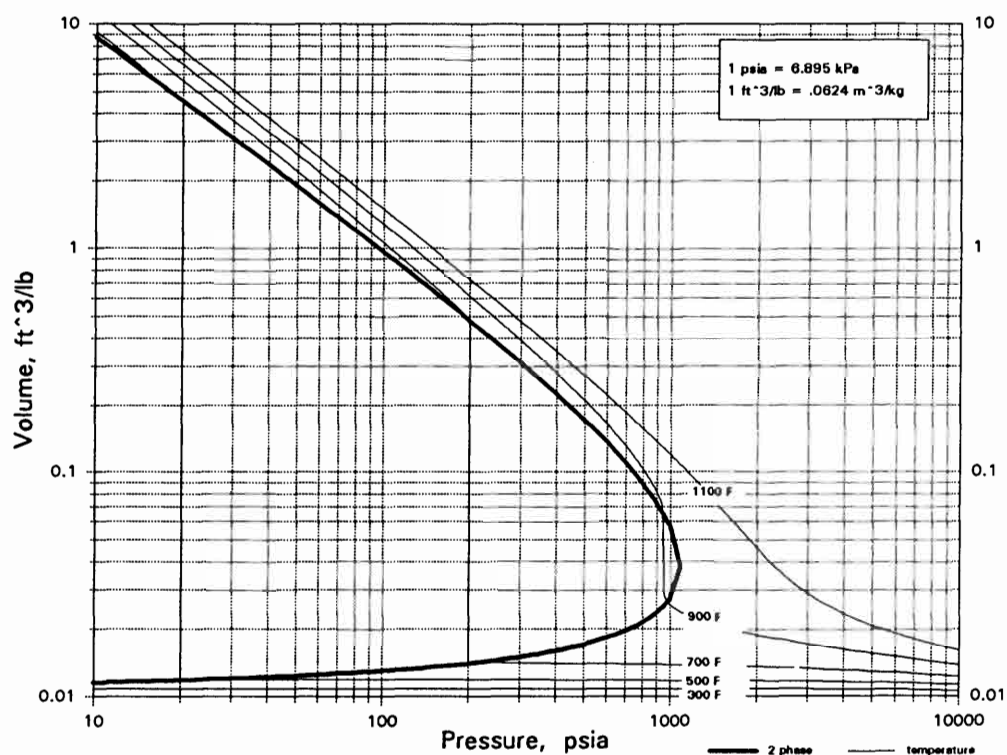
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PHENOL



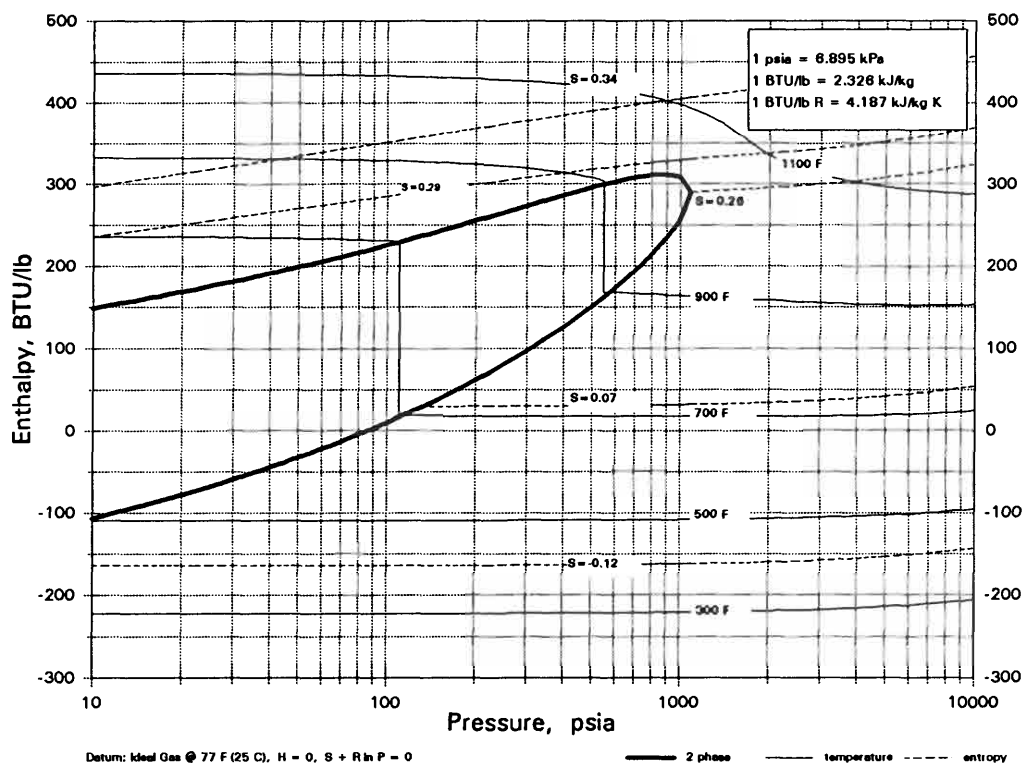
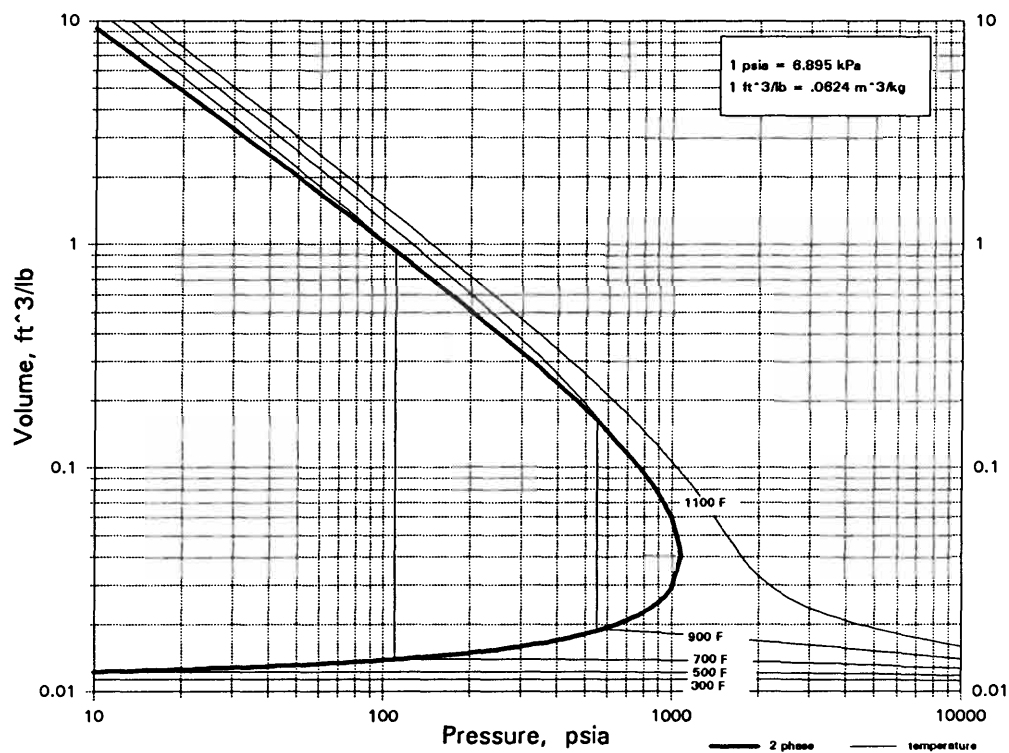
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1-2-BENZENEDIOL



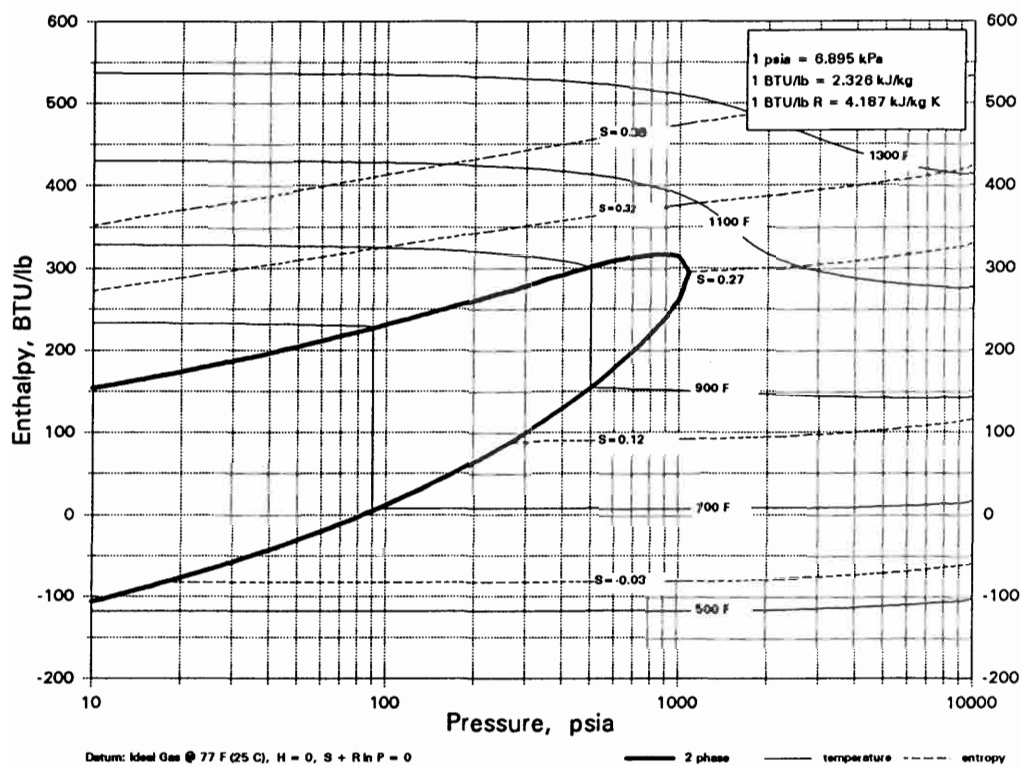
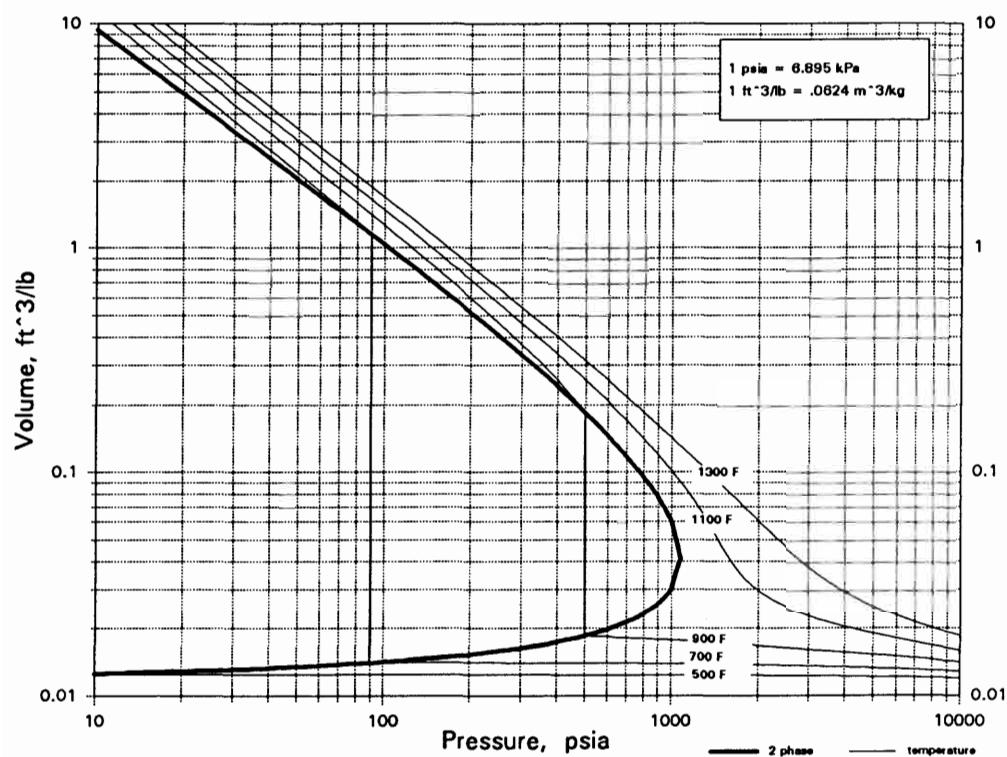
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1-3-BENZENEDIOL



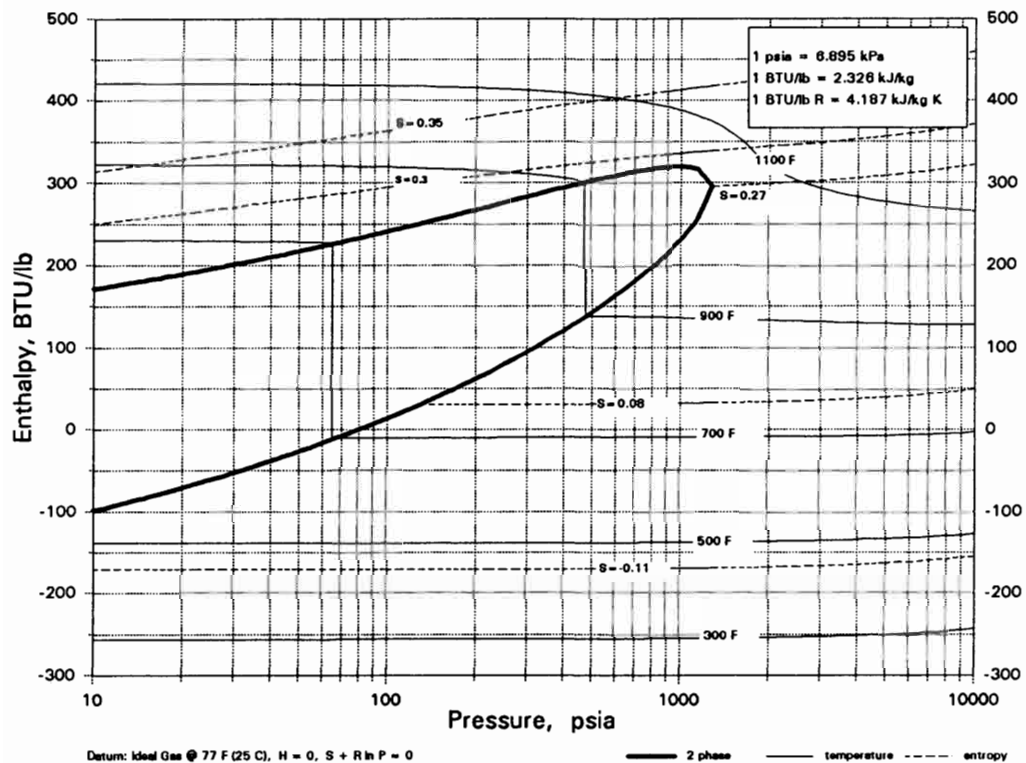
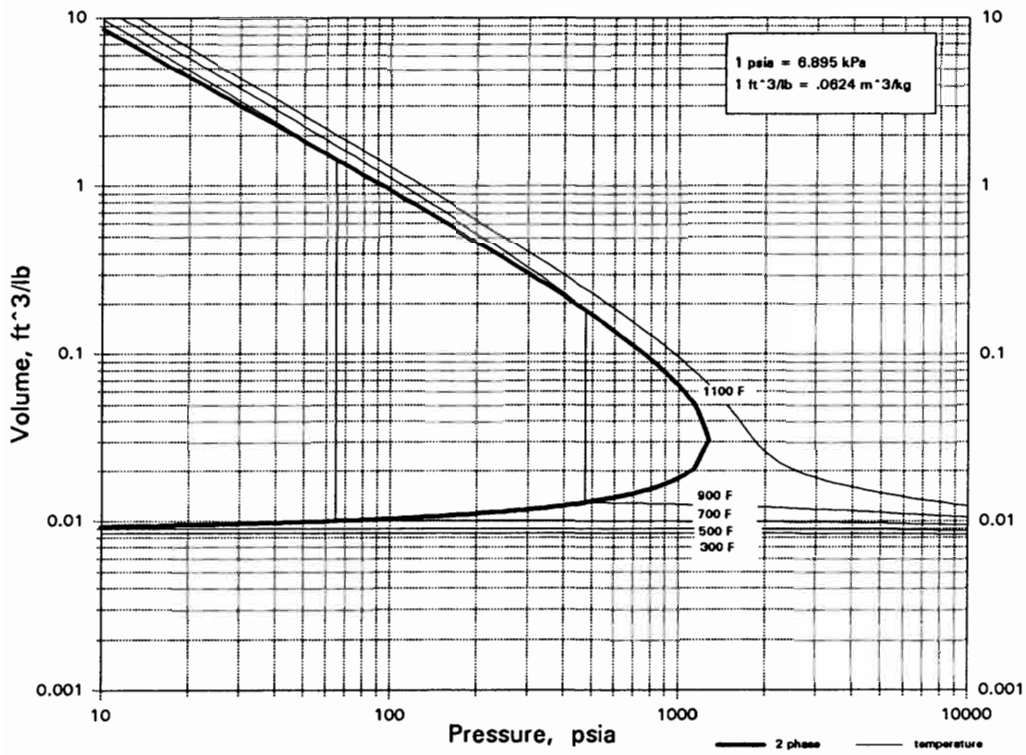
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p-HYDROQUINONE



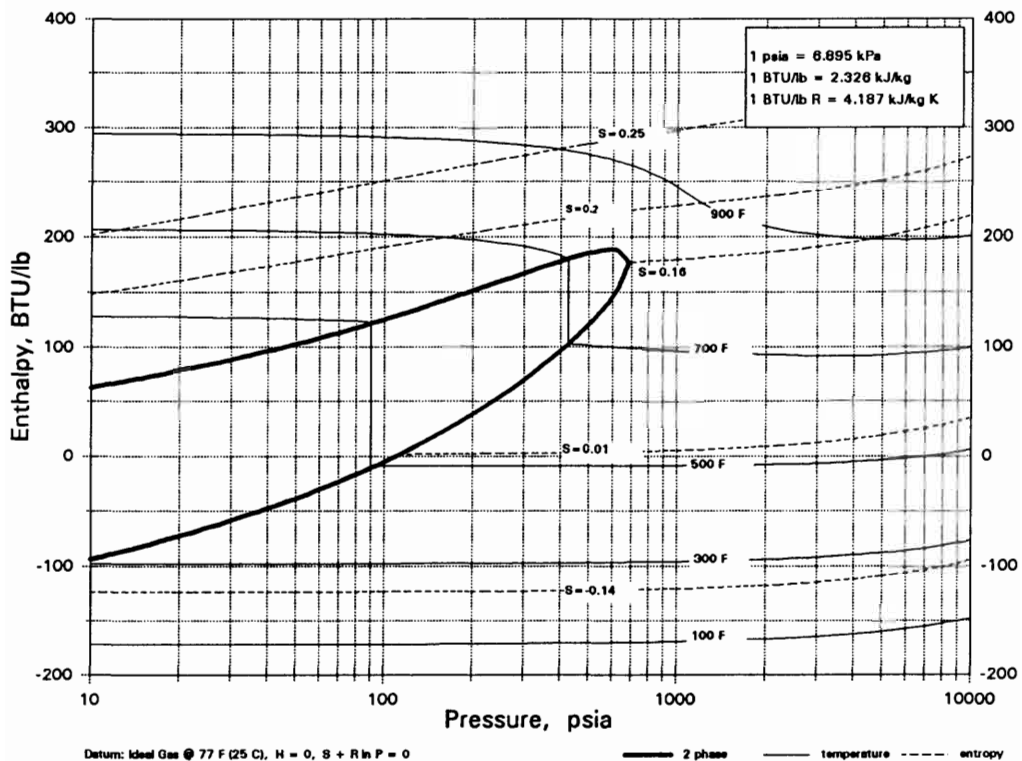
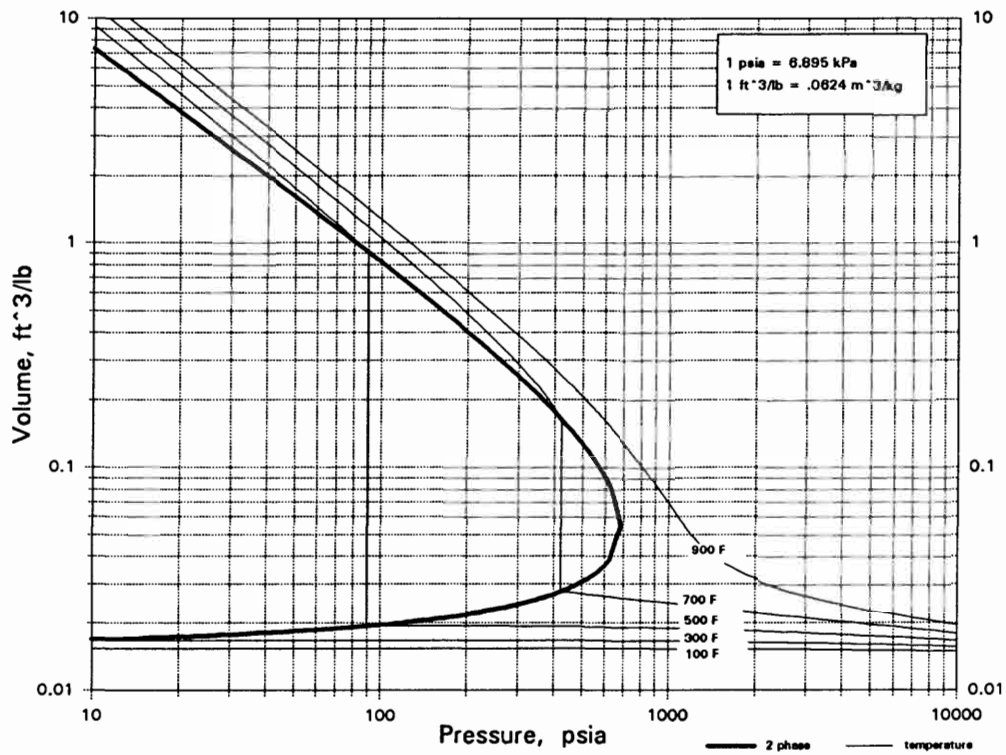
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1-2-3-BENZENETRIOL



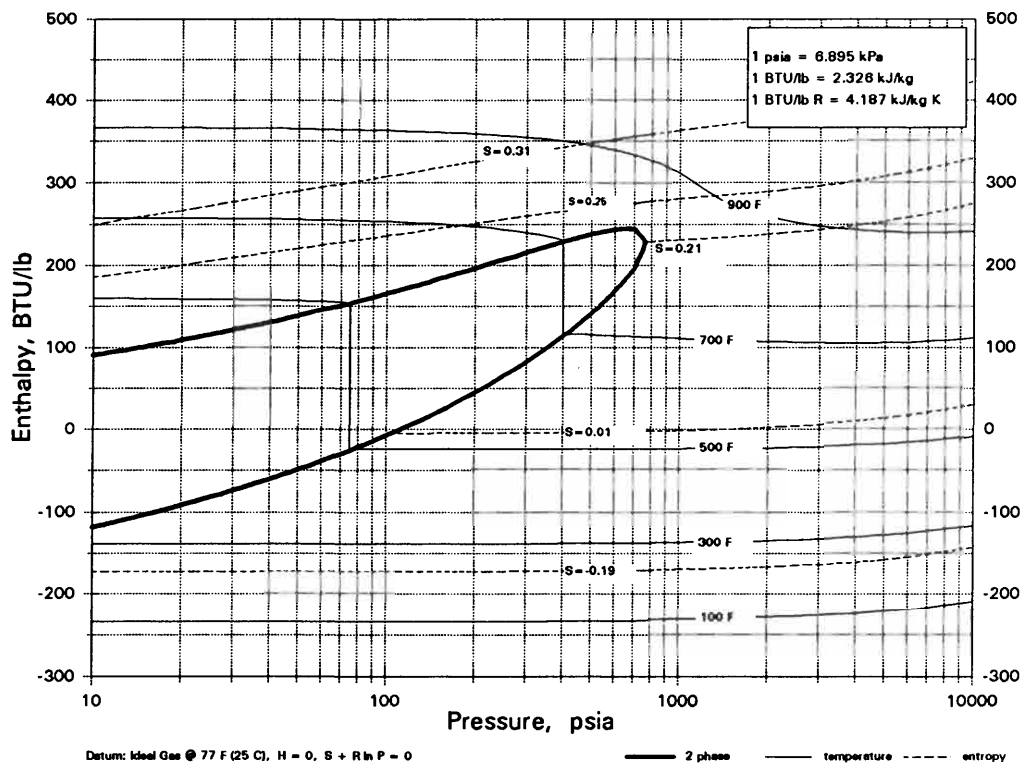
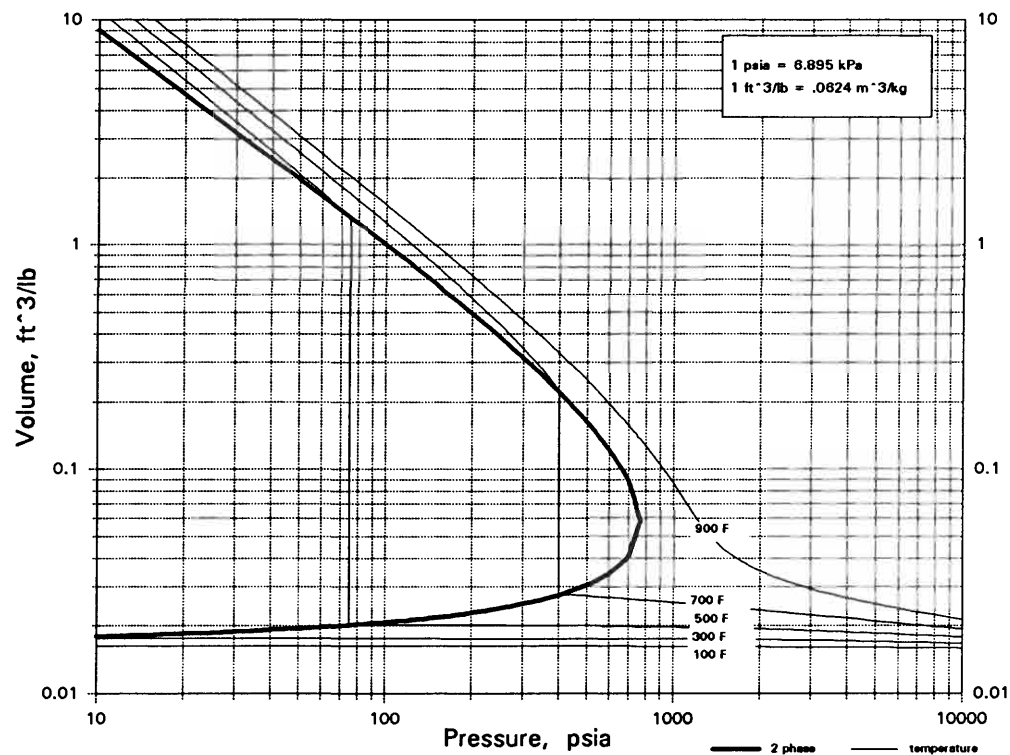
C6H6S

PHENYL MERCAPTAN



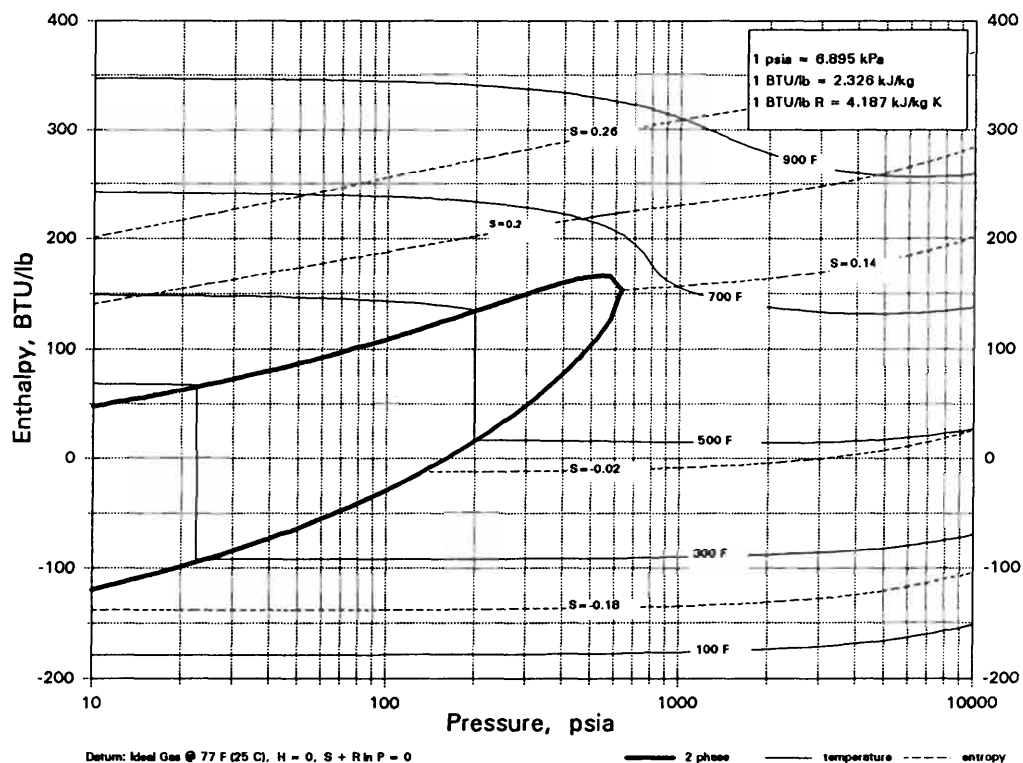
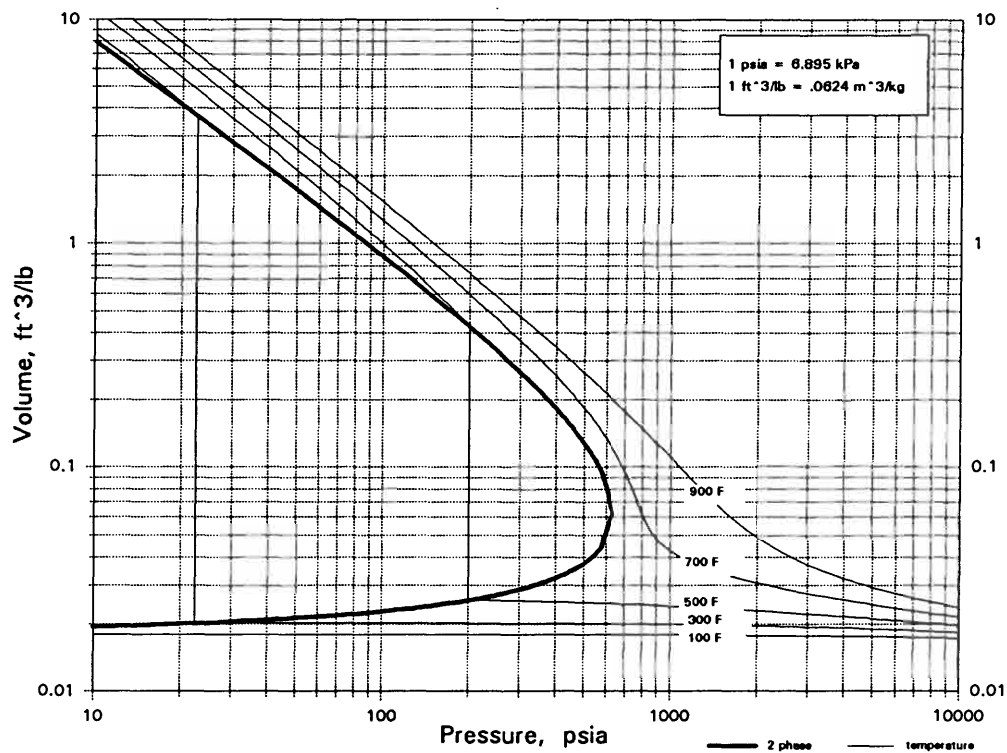
C6H7N

ANILINE



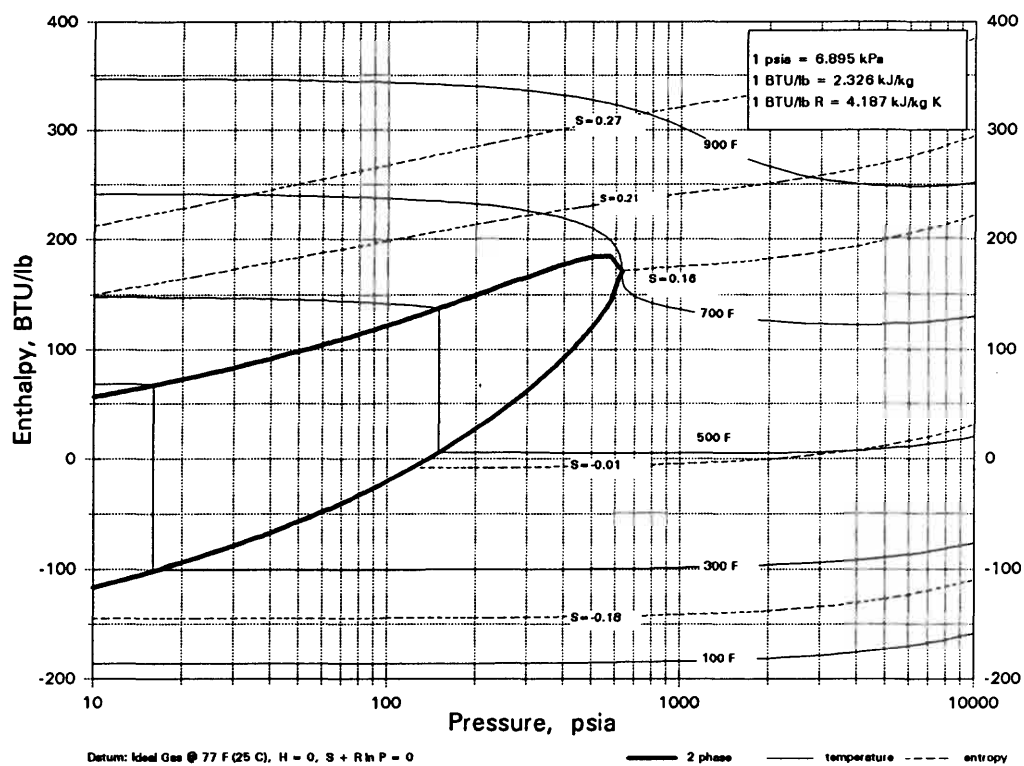
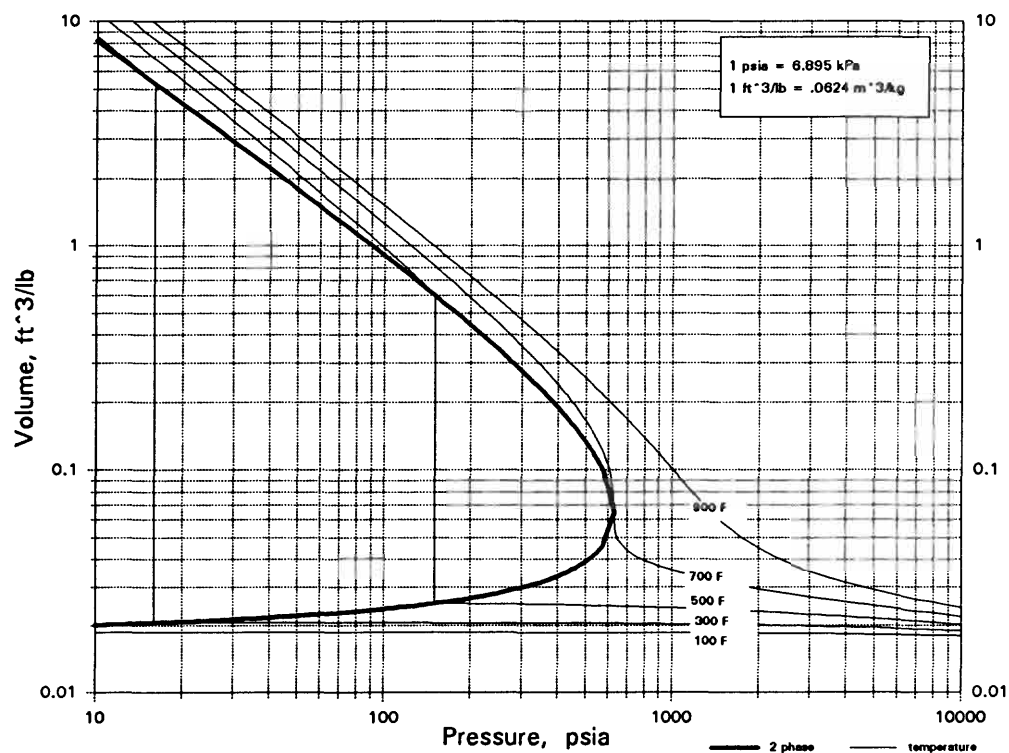
C6H7N

2-METHYLPYRIDINE



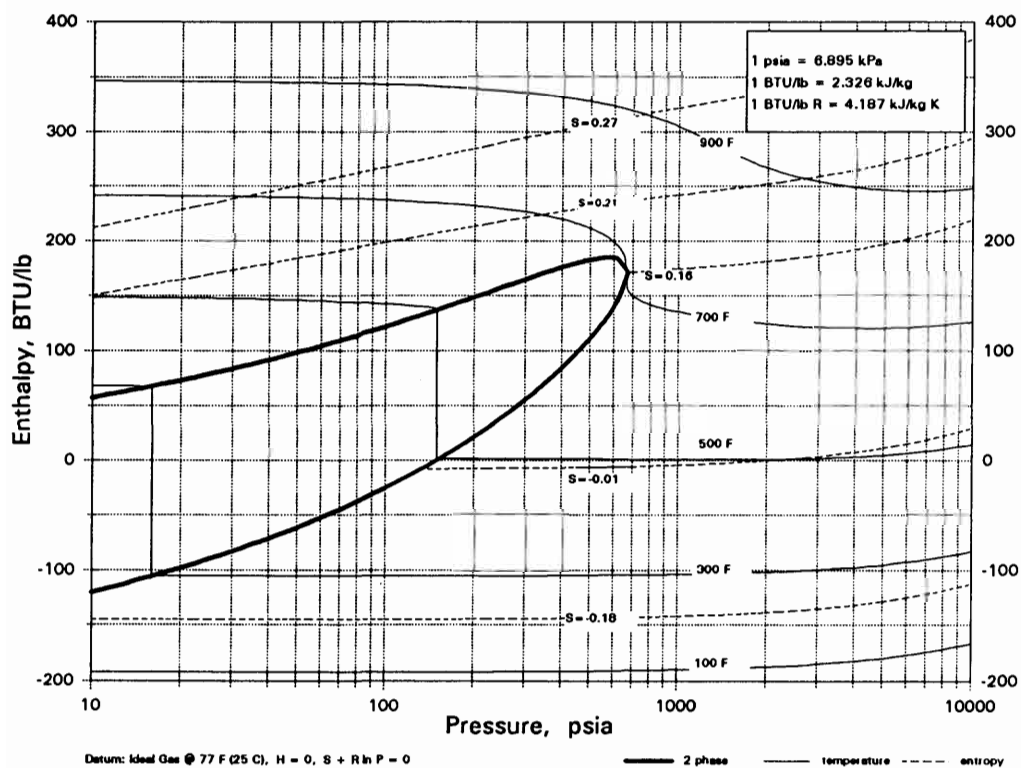
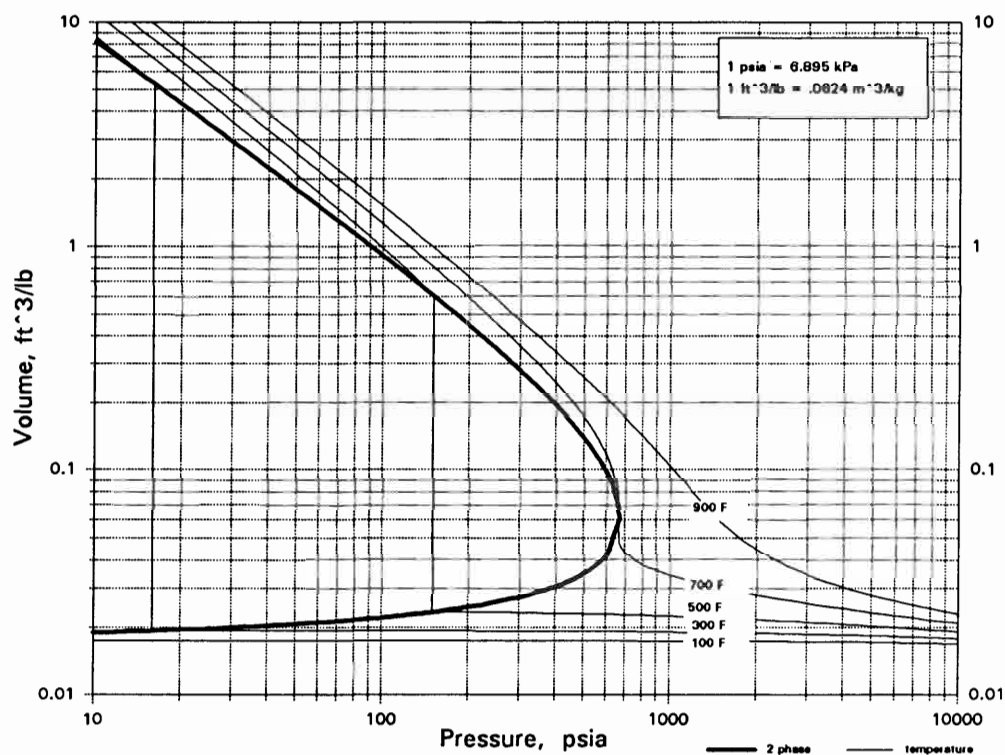
C6H7N

3-METHYLPYRIDINE



C6H7N

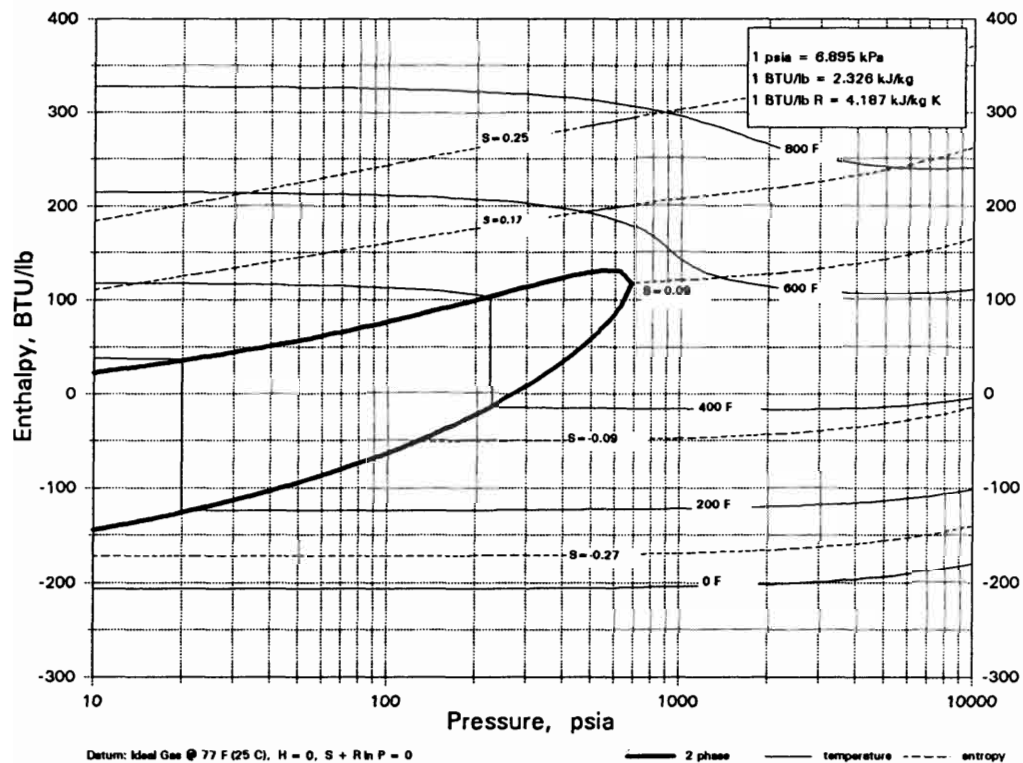
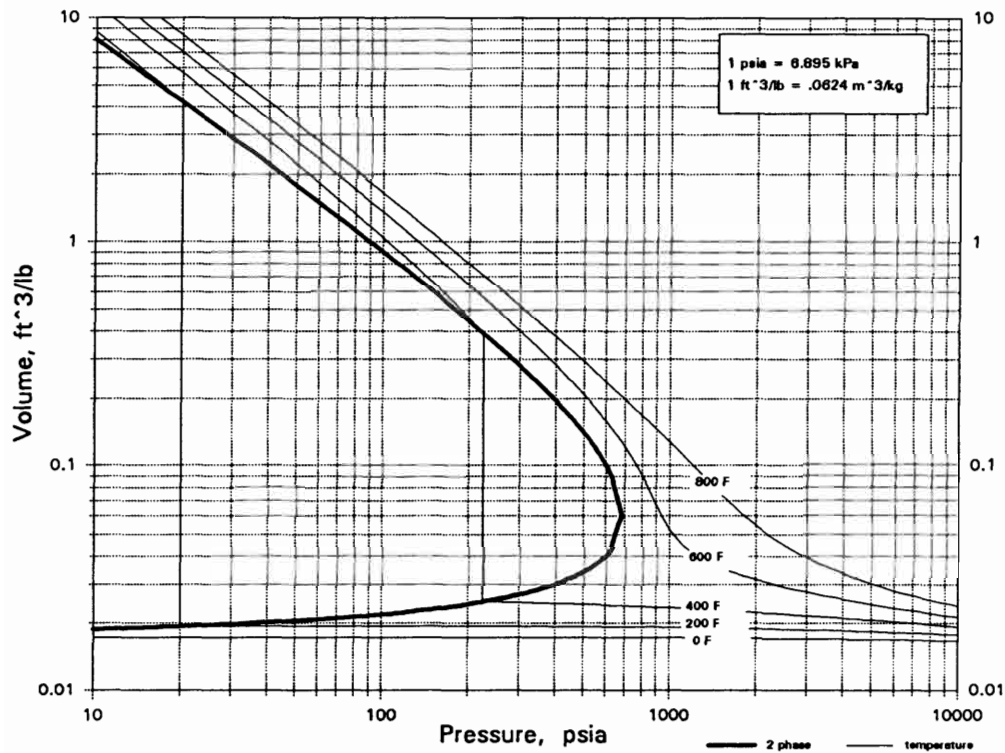
4-METHYLPYRIDINE



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

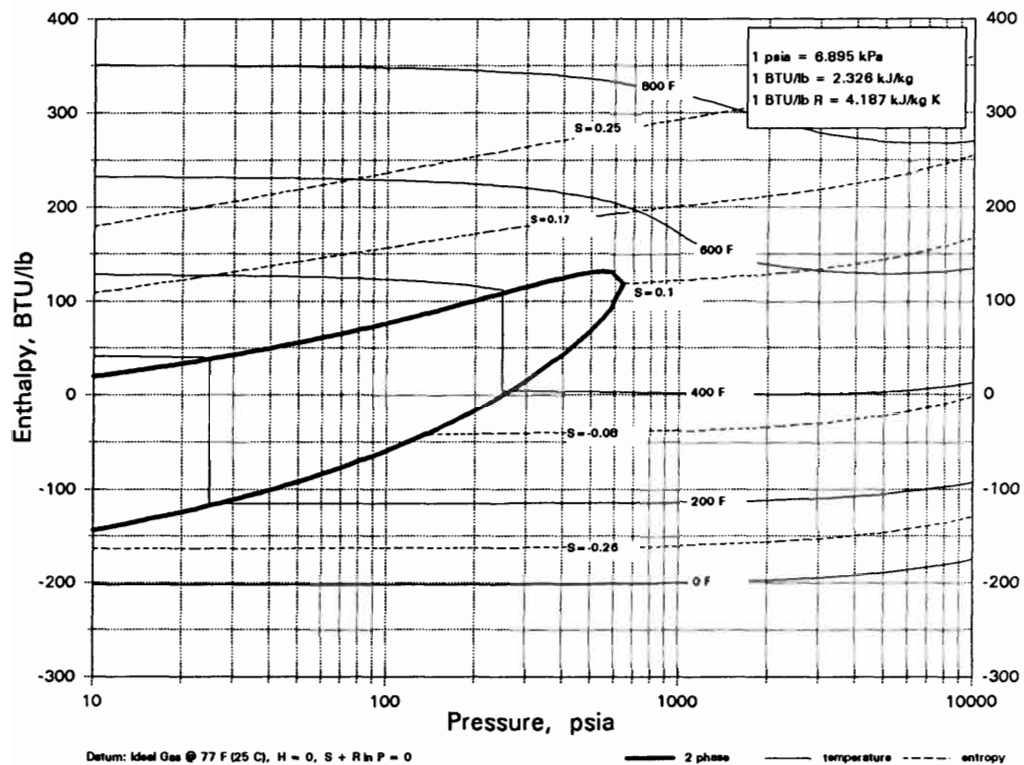
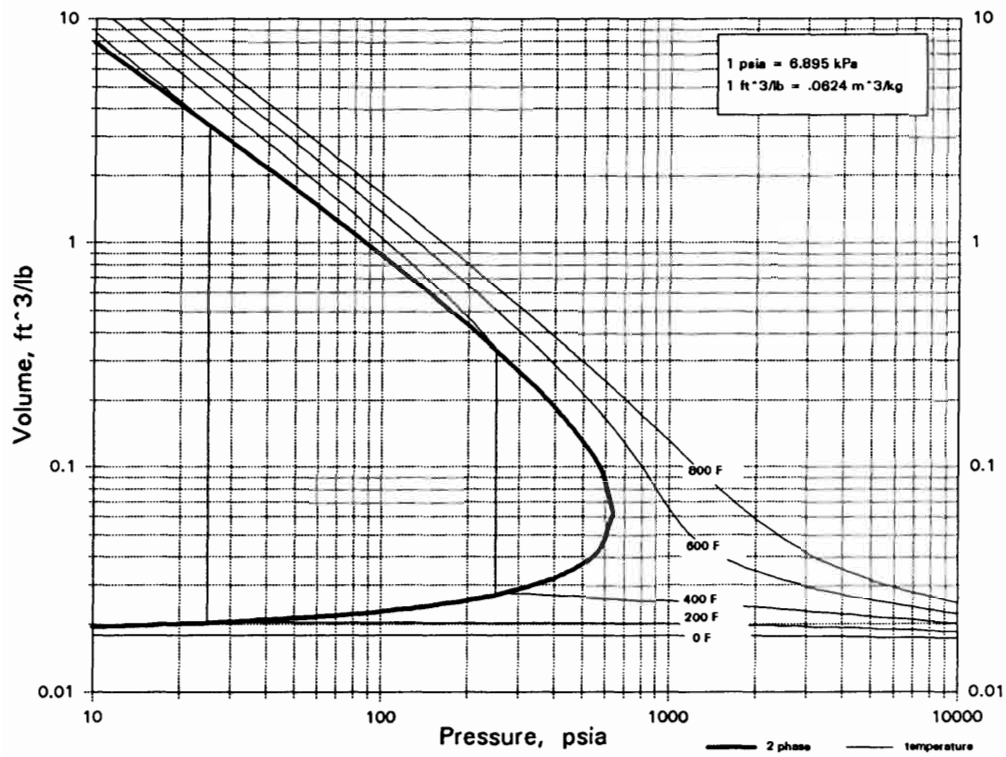
C6H8

1-3-CYCLOHEXADIENE



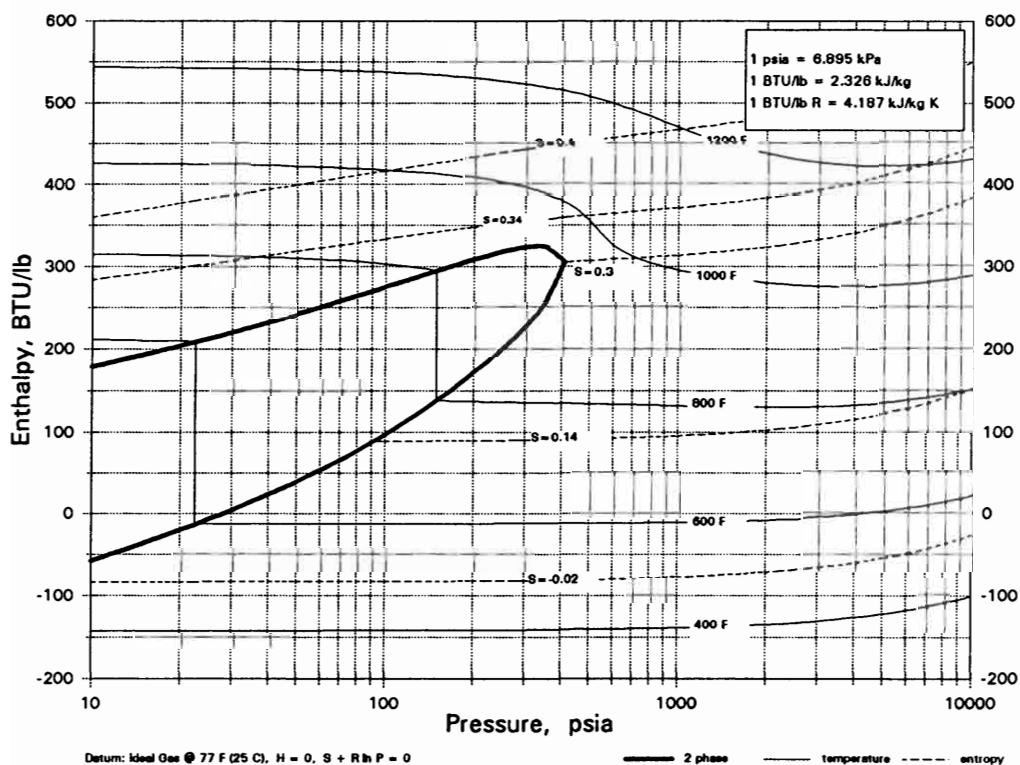
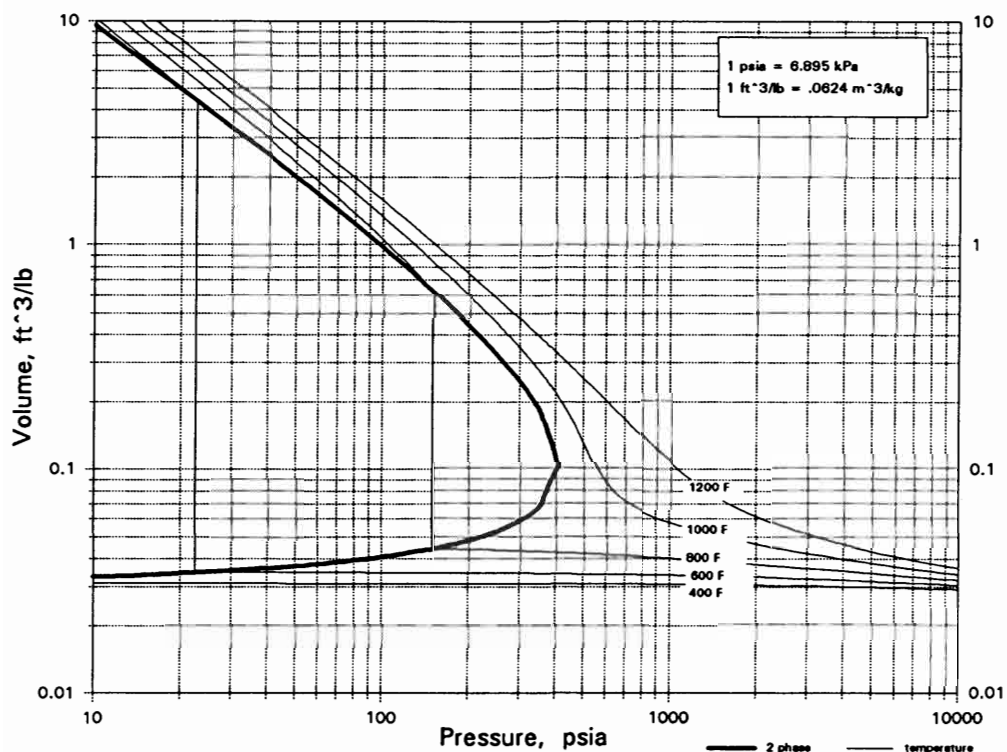
C6H8

METHYLCYCLOPENTADIENE



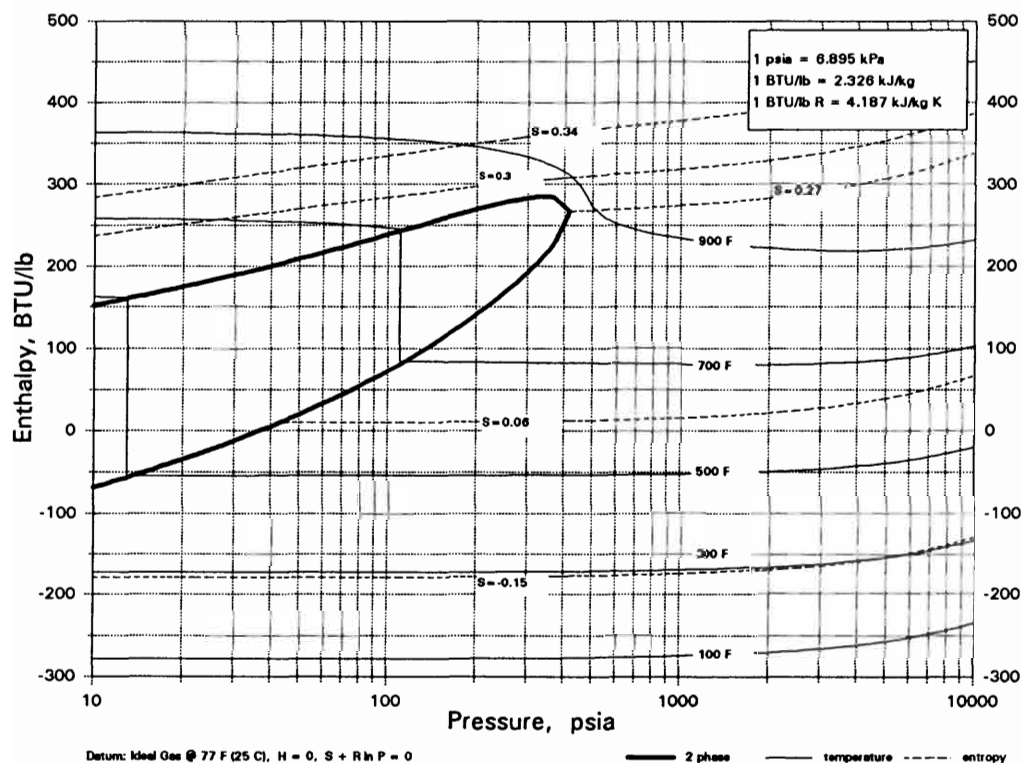
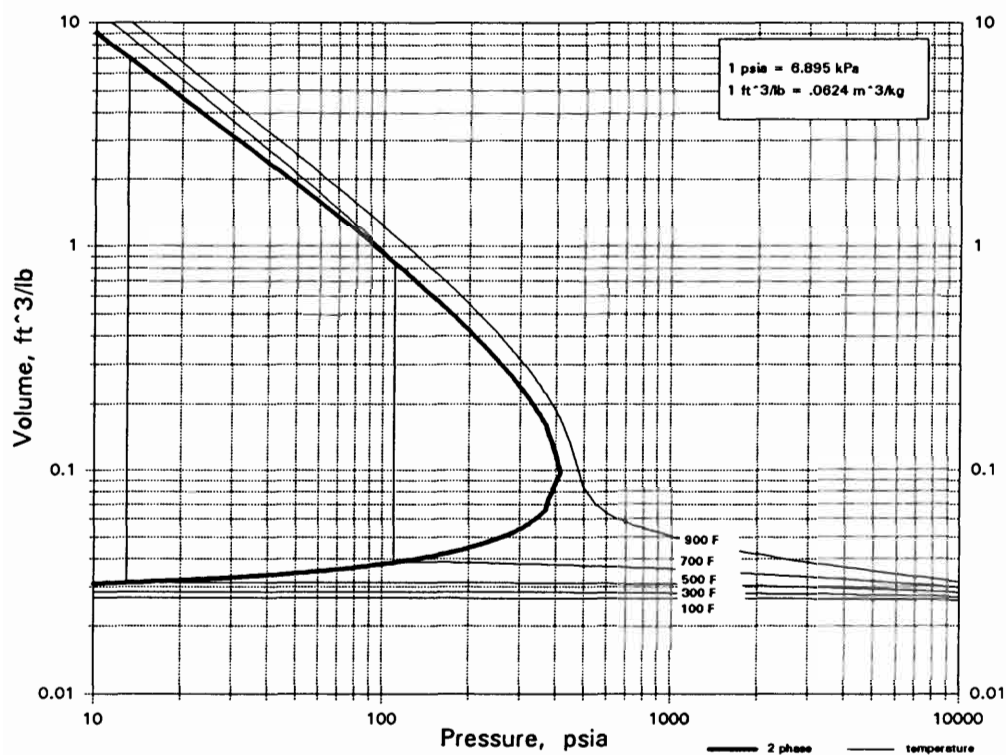
C6H8N2

ADIPONITRILE



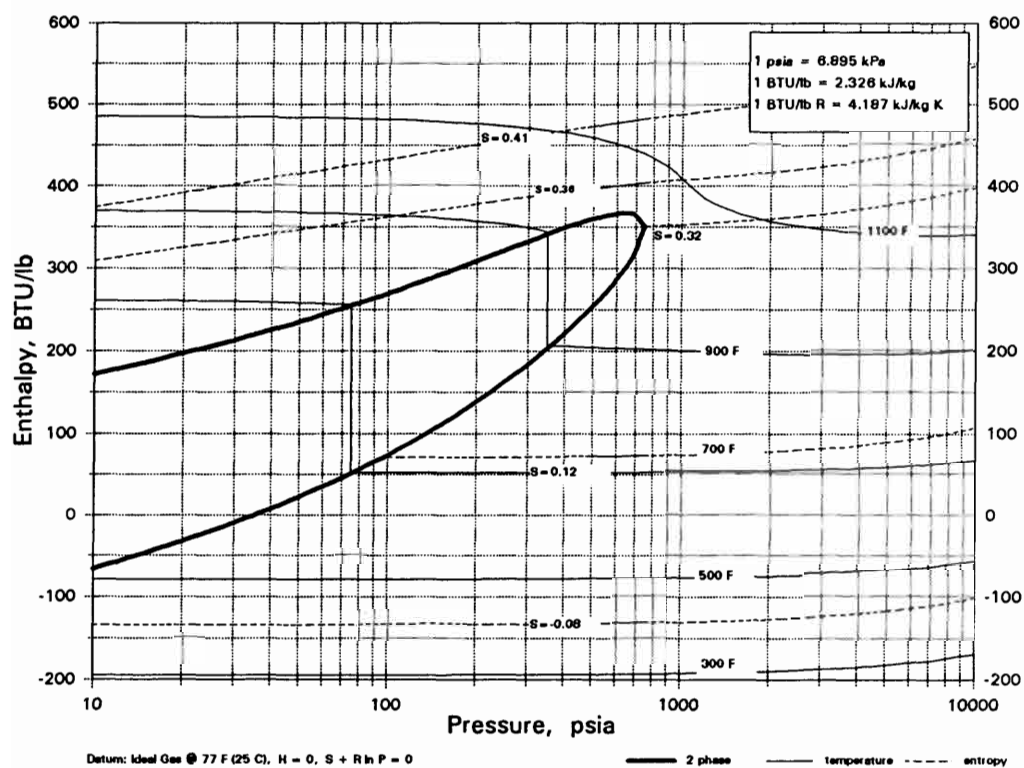
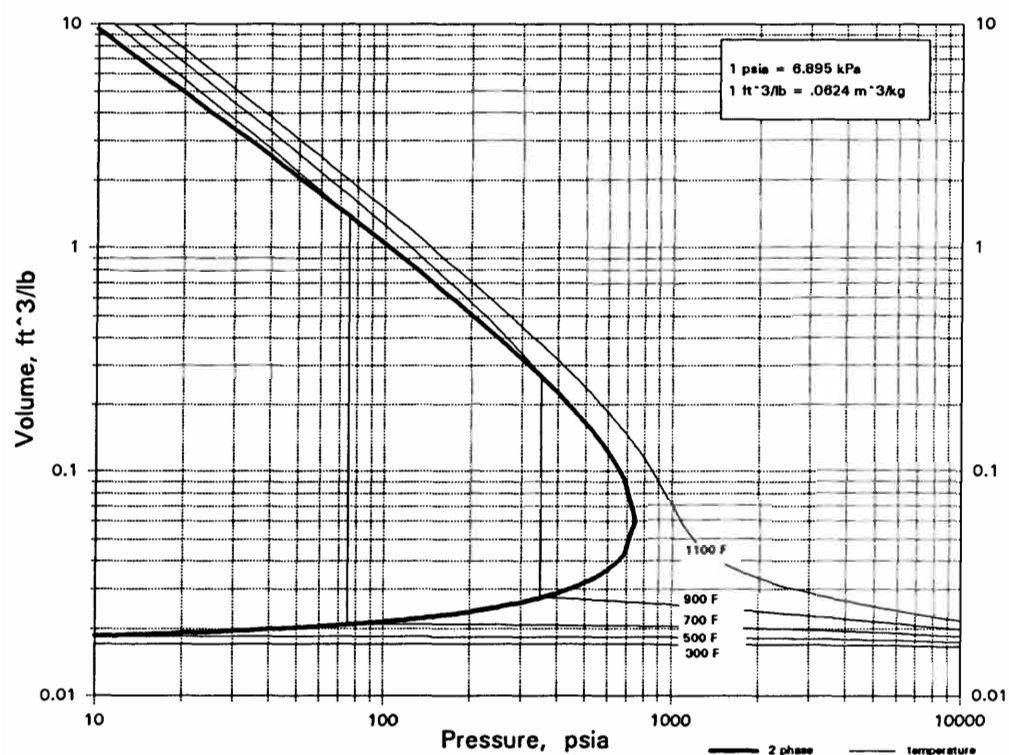
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METHYLGLUTARONITRILE



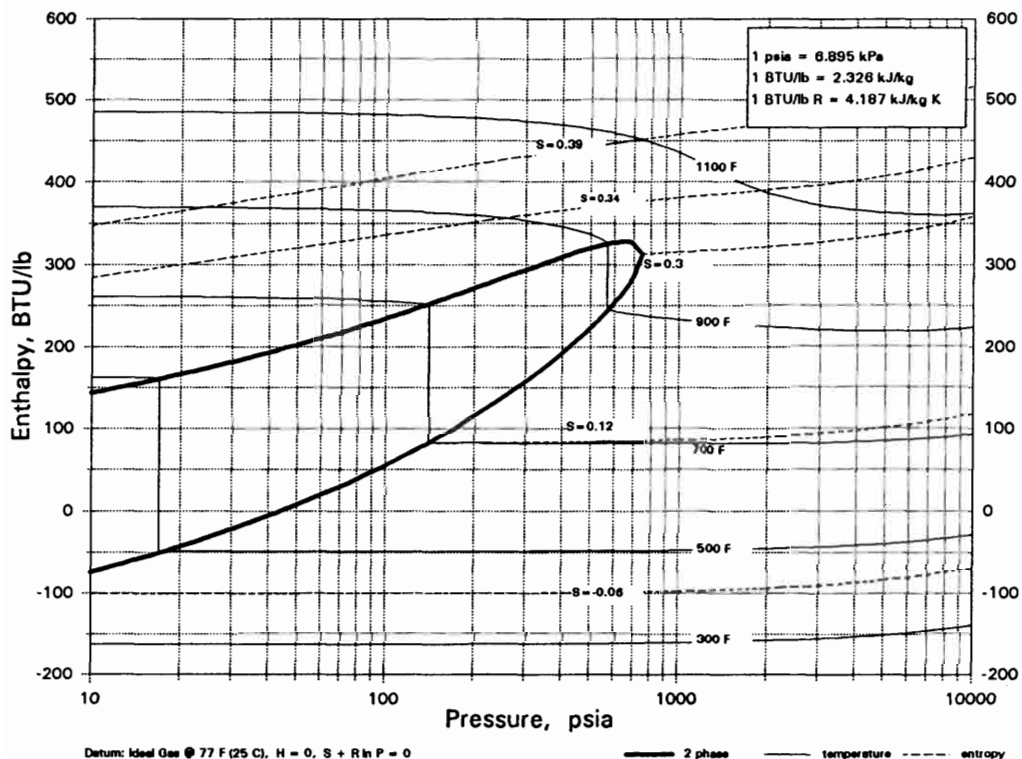
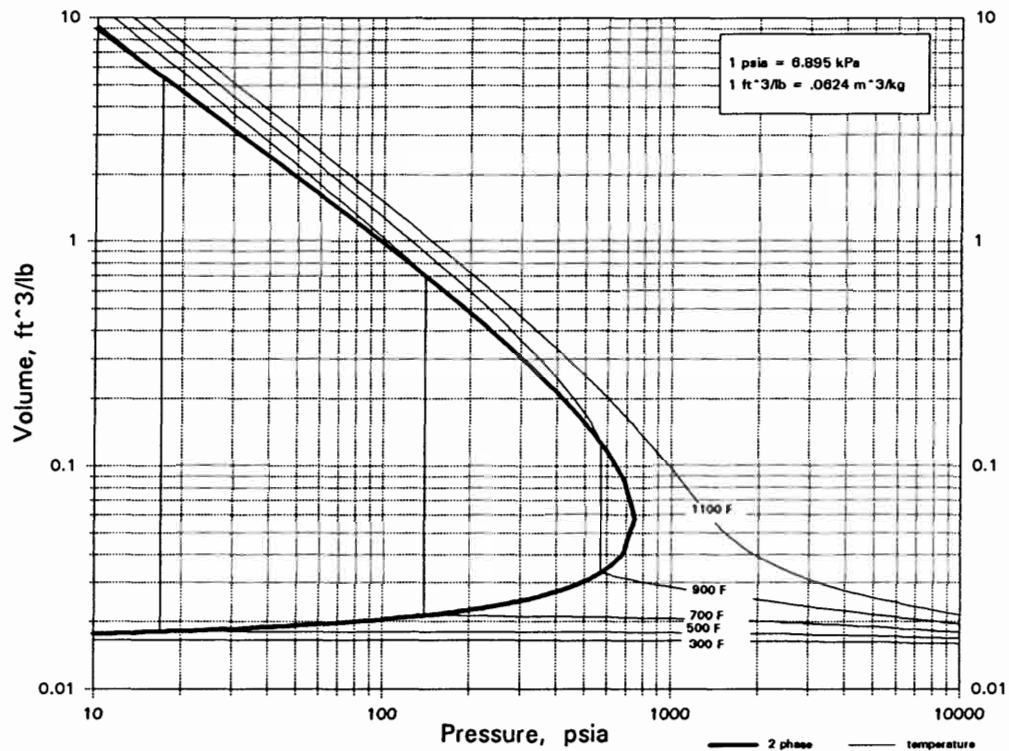
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m-PHENYLENEDIAMINE



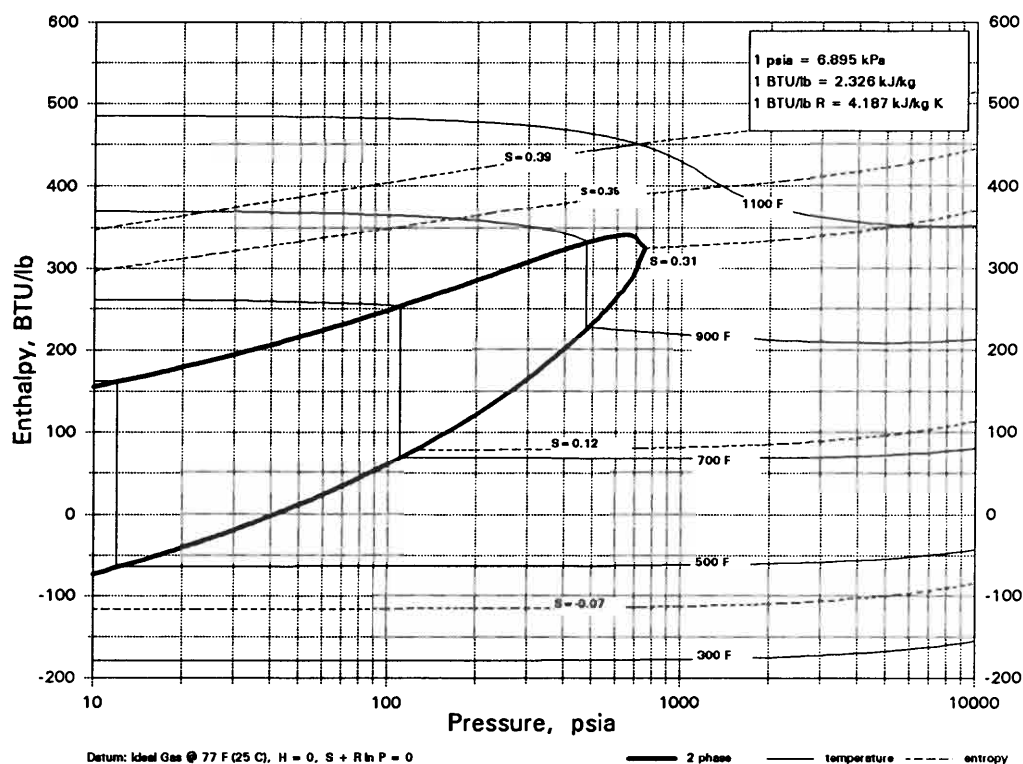
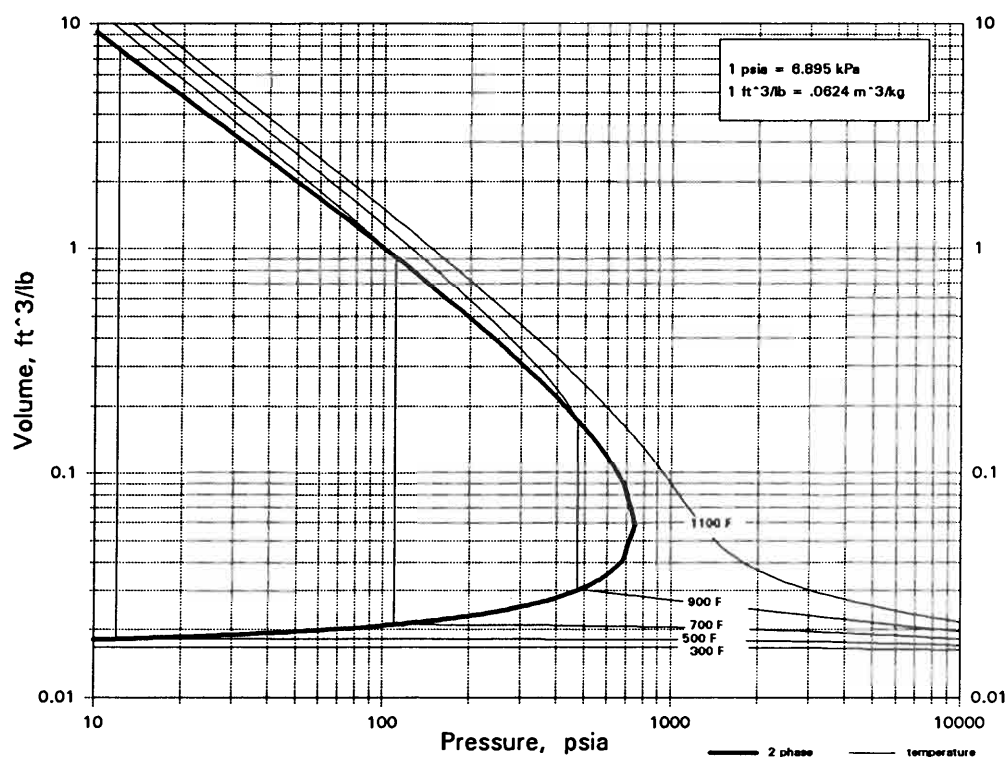
C6H8N2

o-PHENYLENEDIAMINE



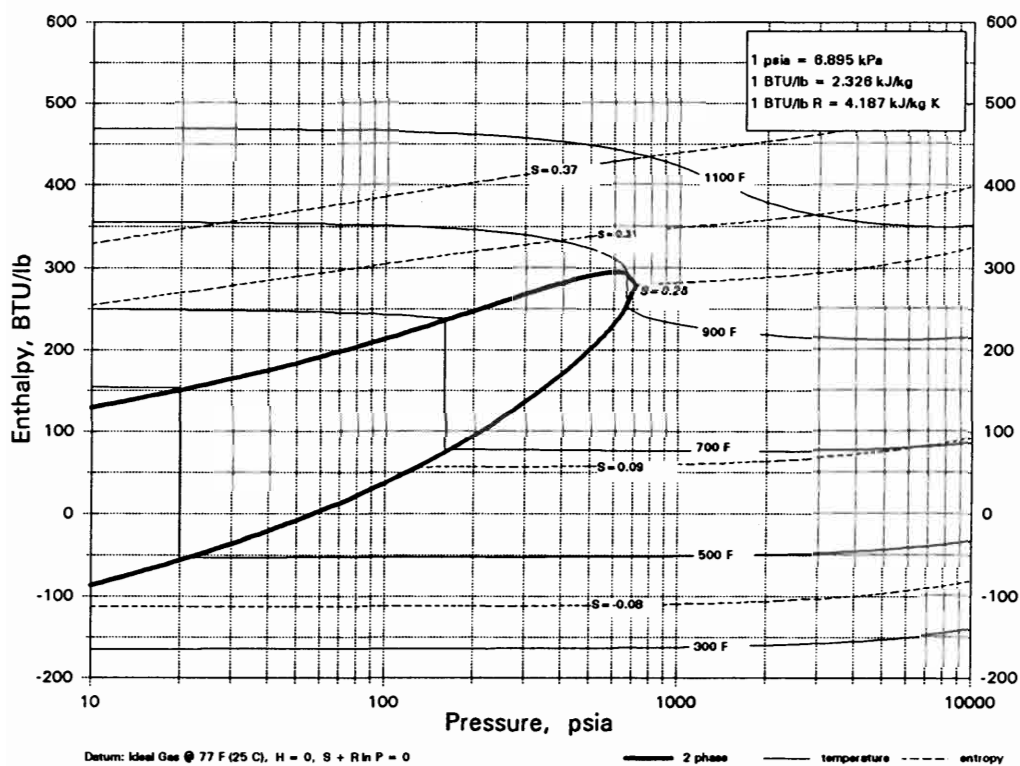
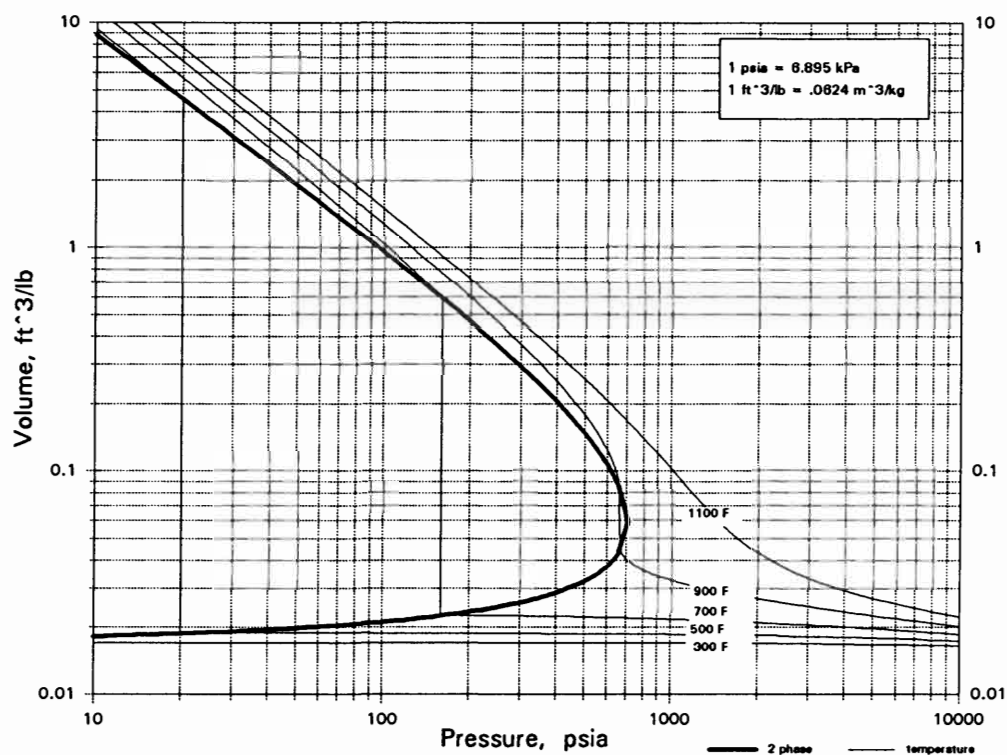
C₆H₈N₂

p-PHENYLENEDIAMINE



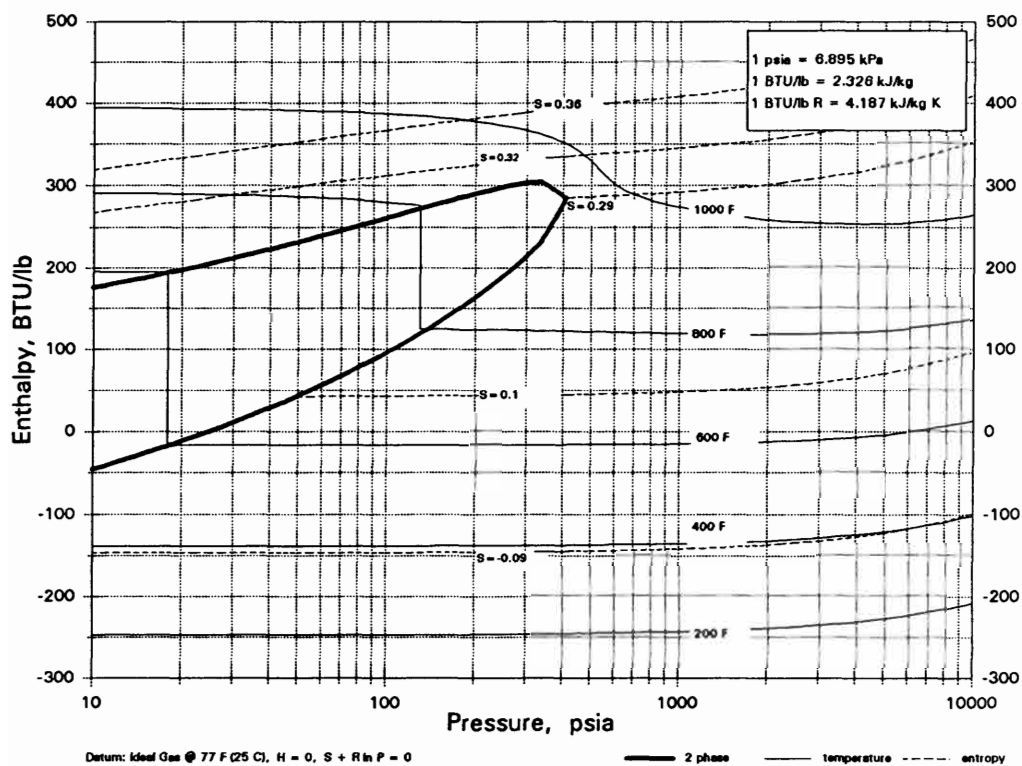
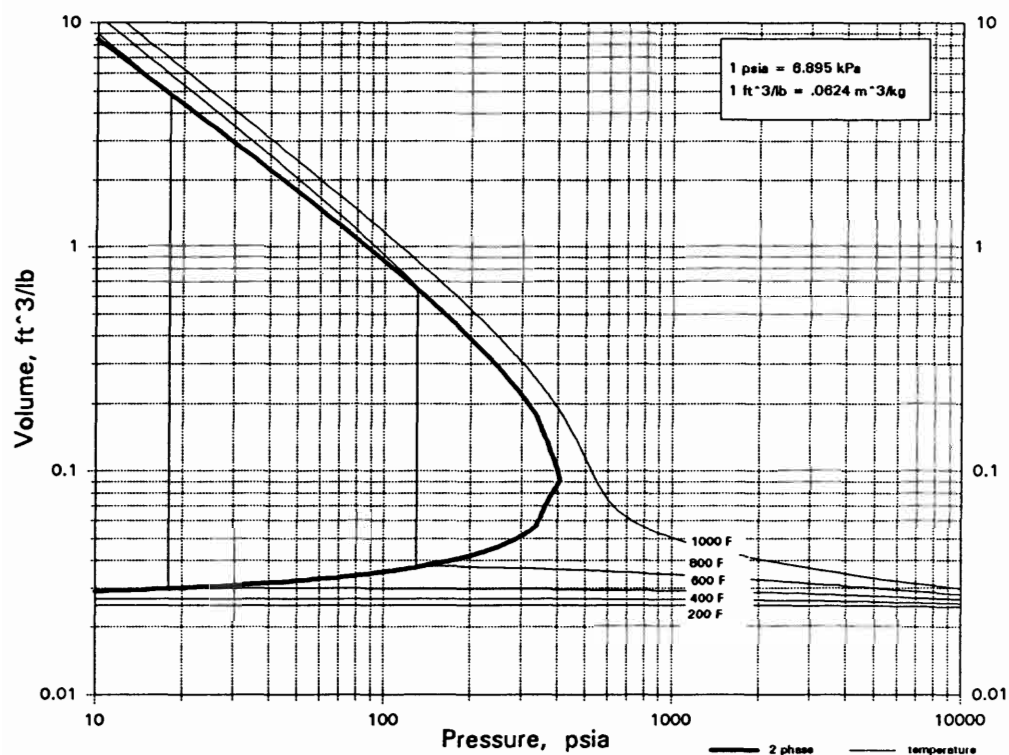
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PHENYLHYDRAZINE



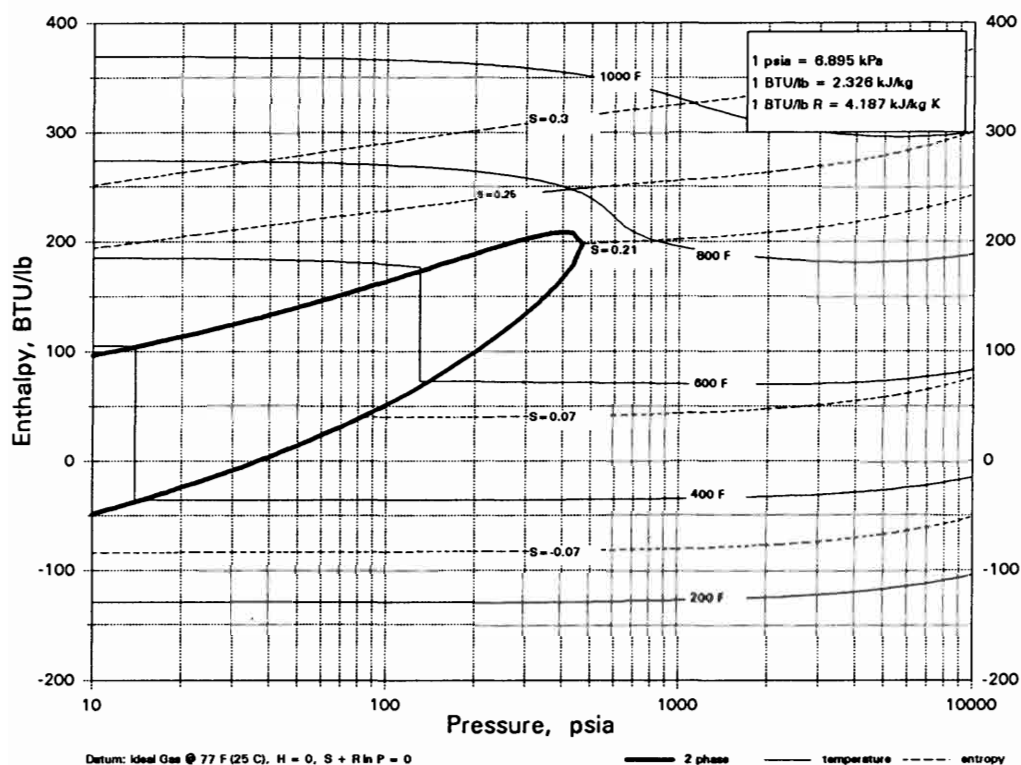
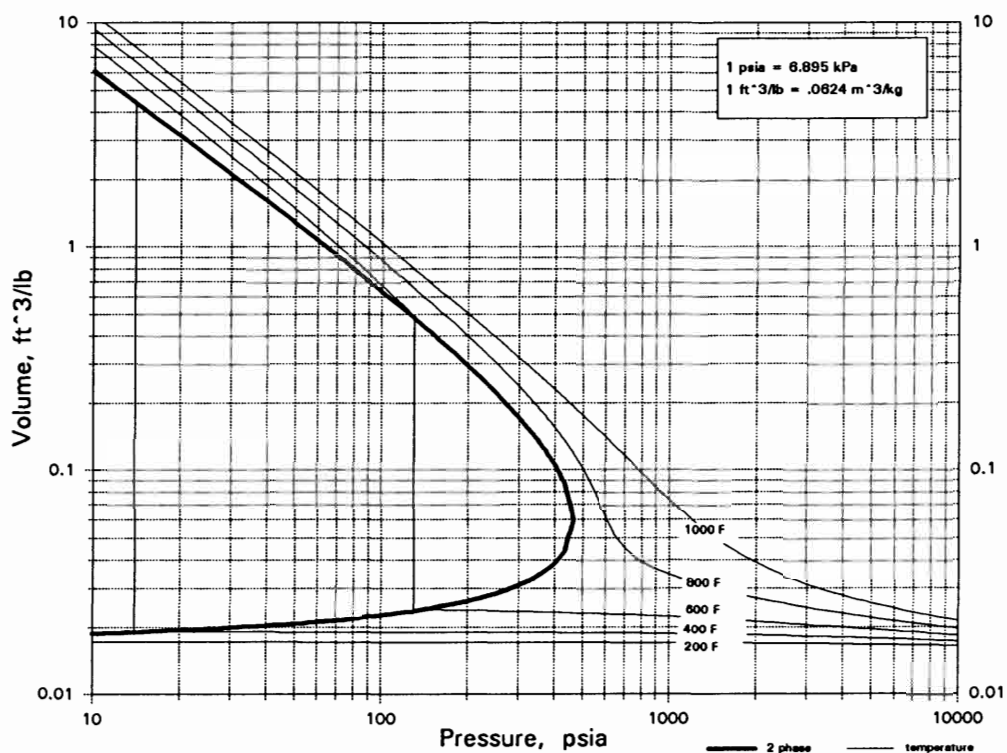
C6H8N2O

BIS(CYANOETHYL)ETHER



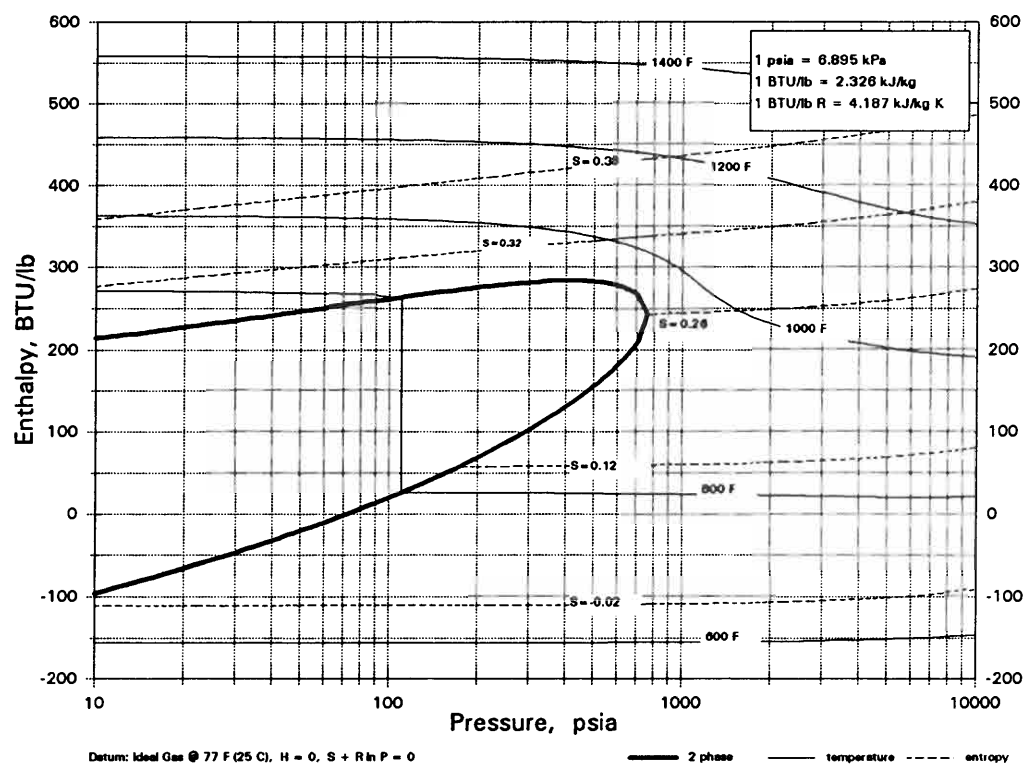
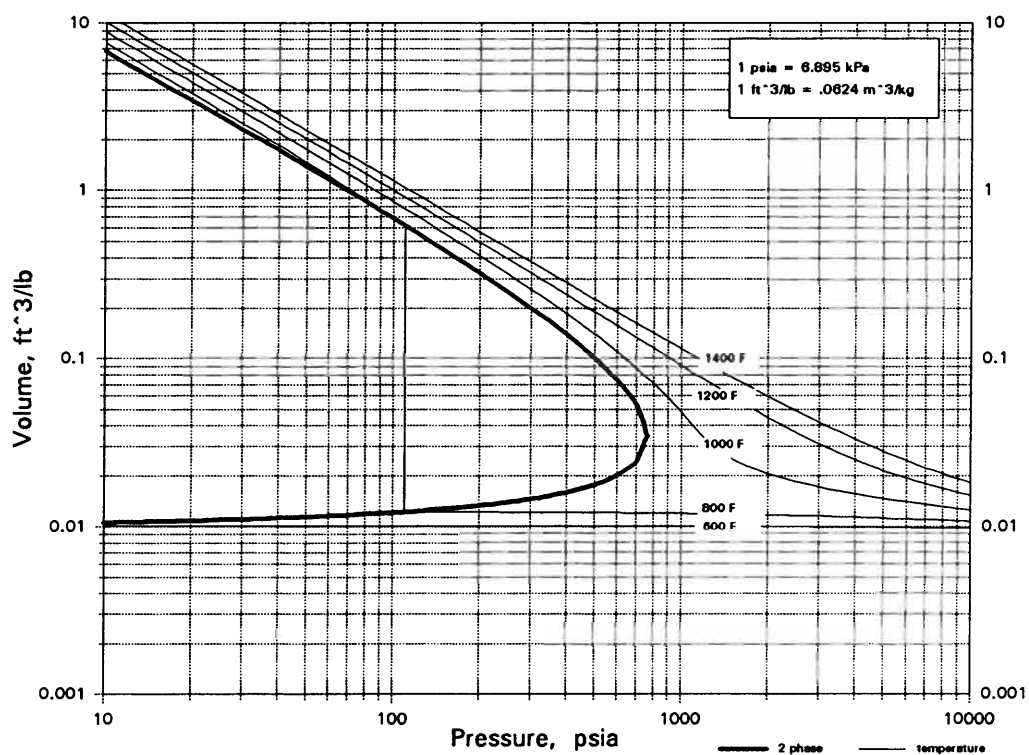
C6H8O4

DIMETHYL MALEATE



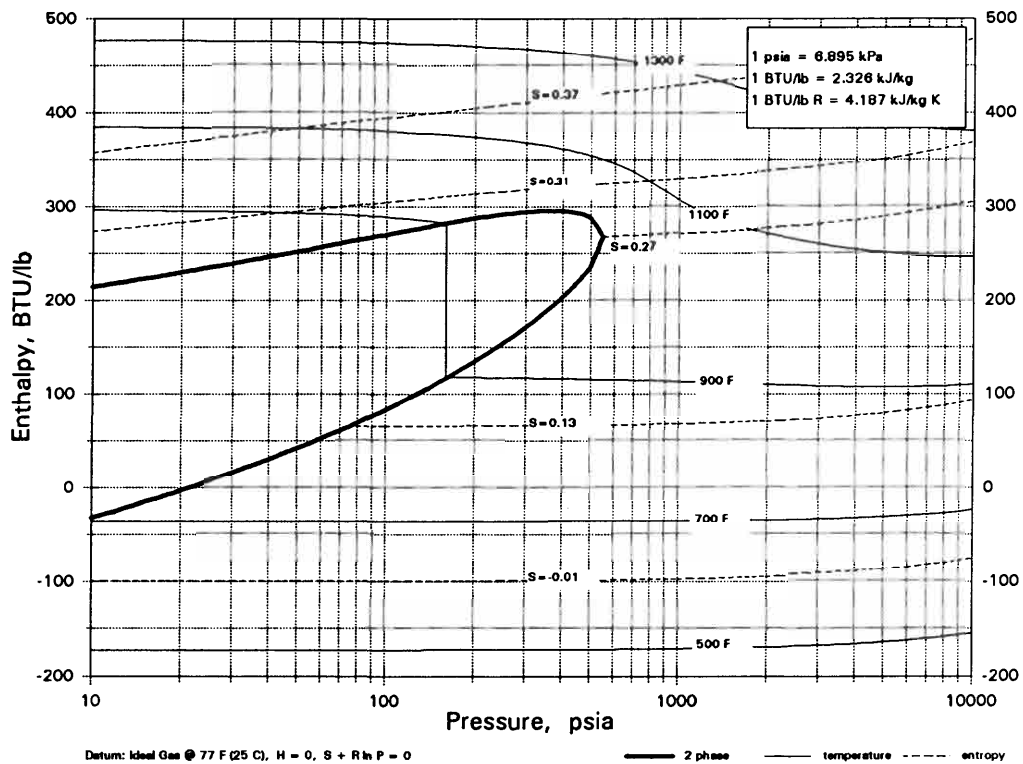
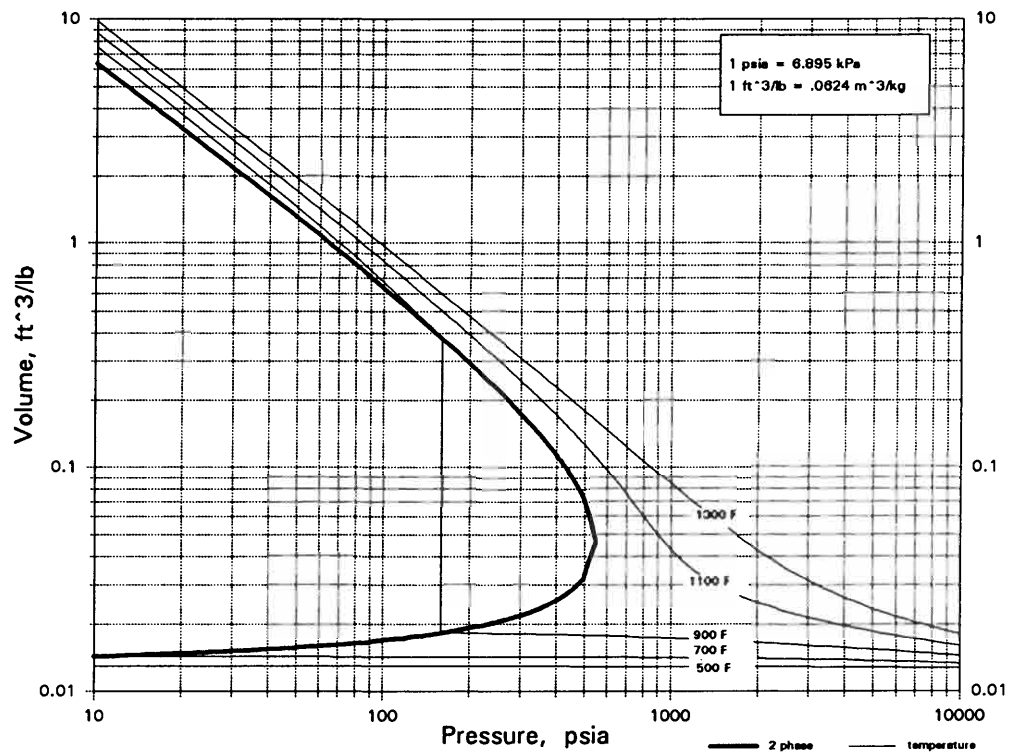
C6H8O6

ASCORBIC ACID



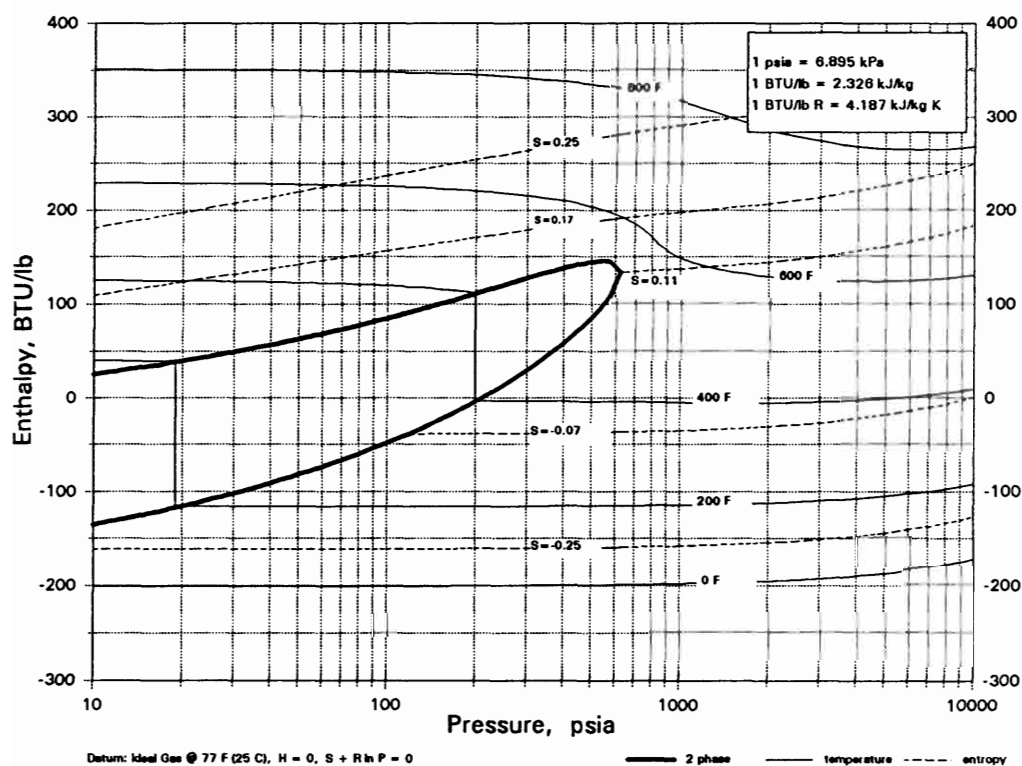
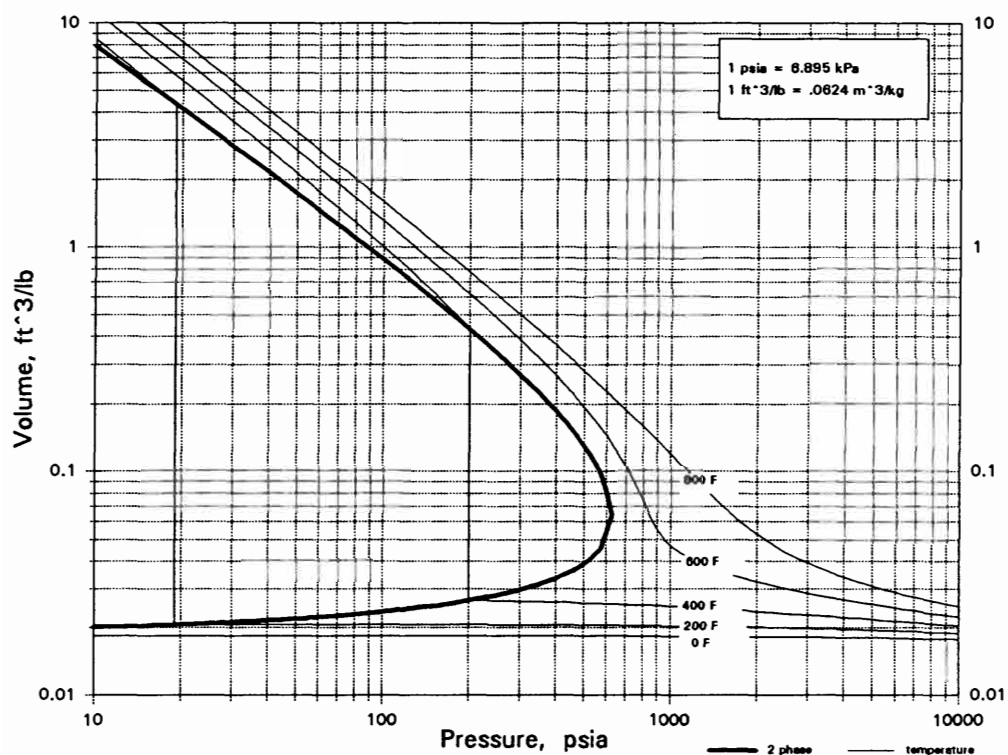
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CITRIC ACID



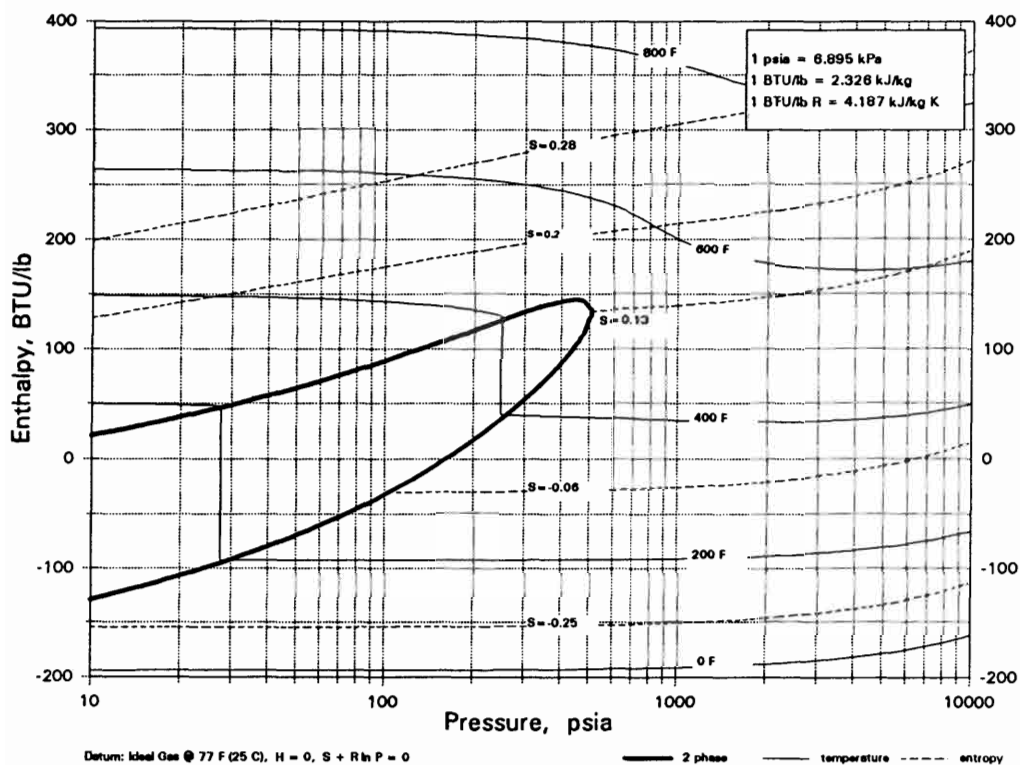
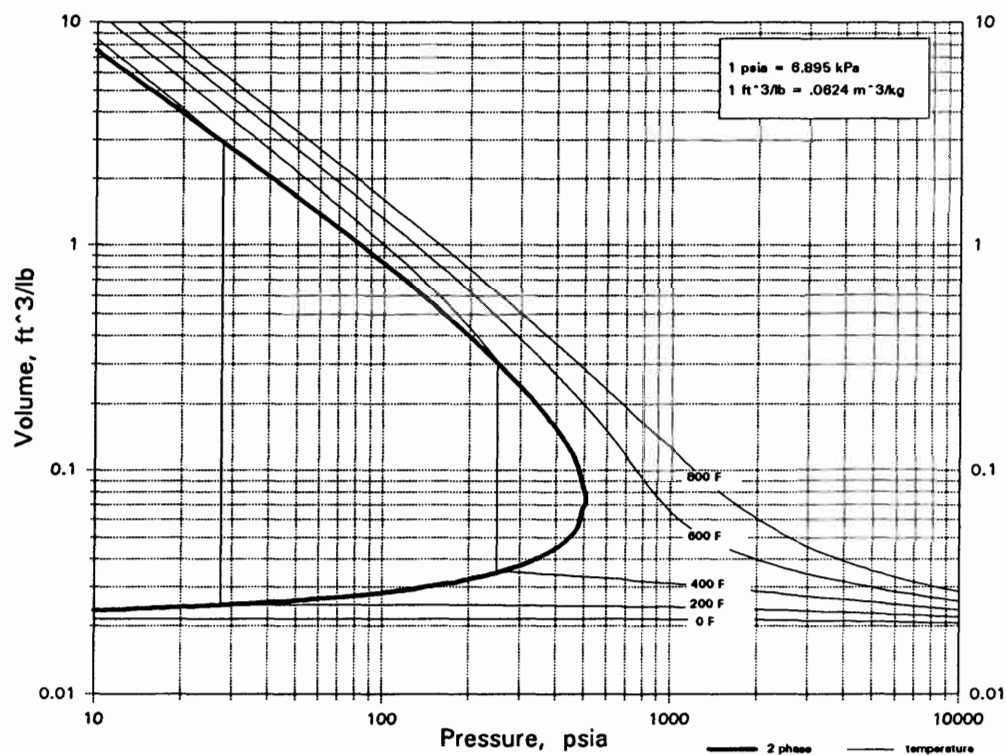
C6H10

CYCLOHEXENE



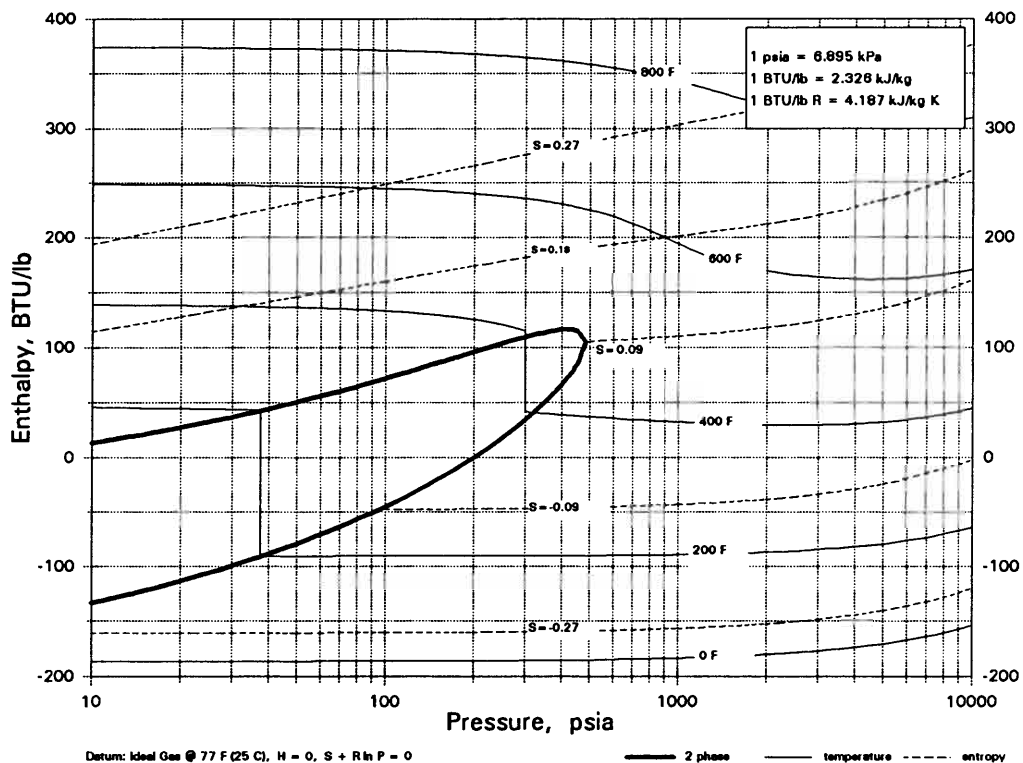
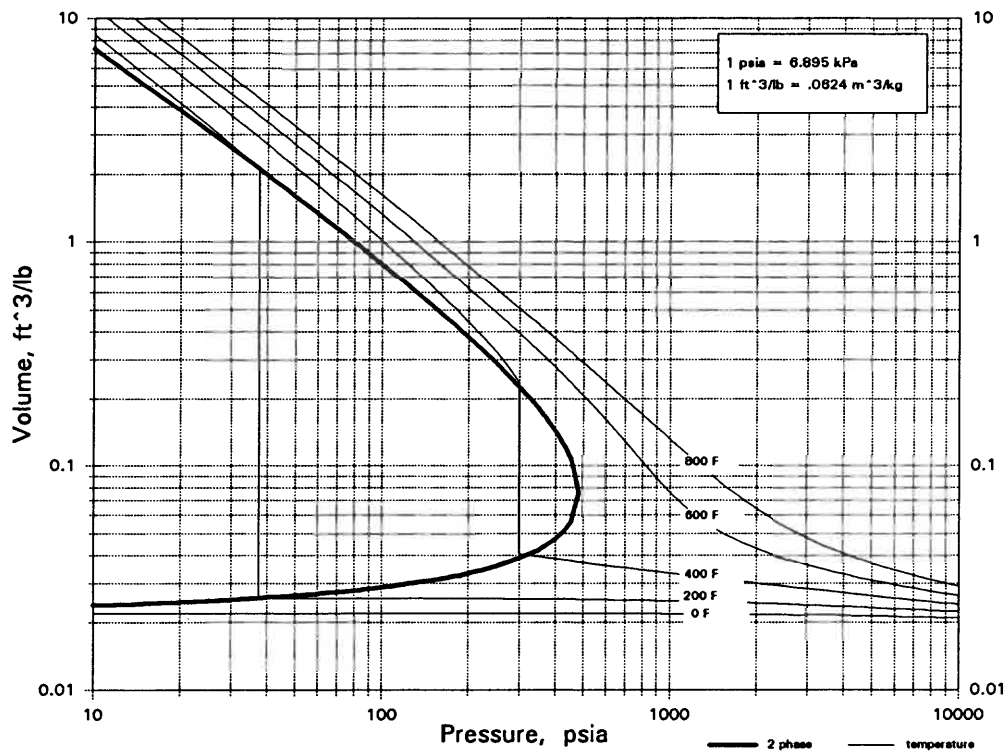
C6H10

2-3-DIMETHYL-1-3-BUTADIENE



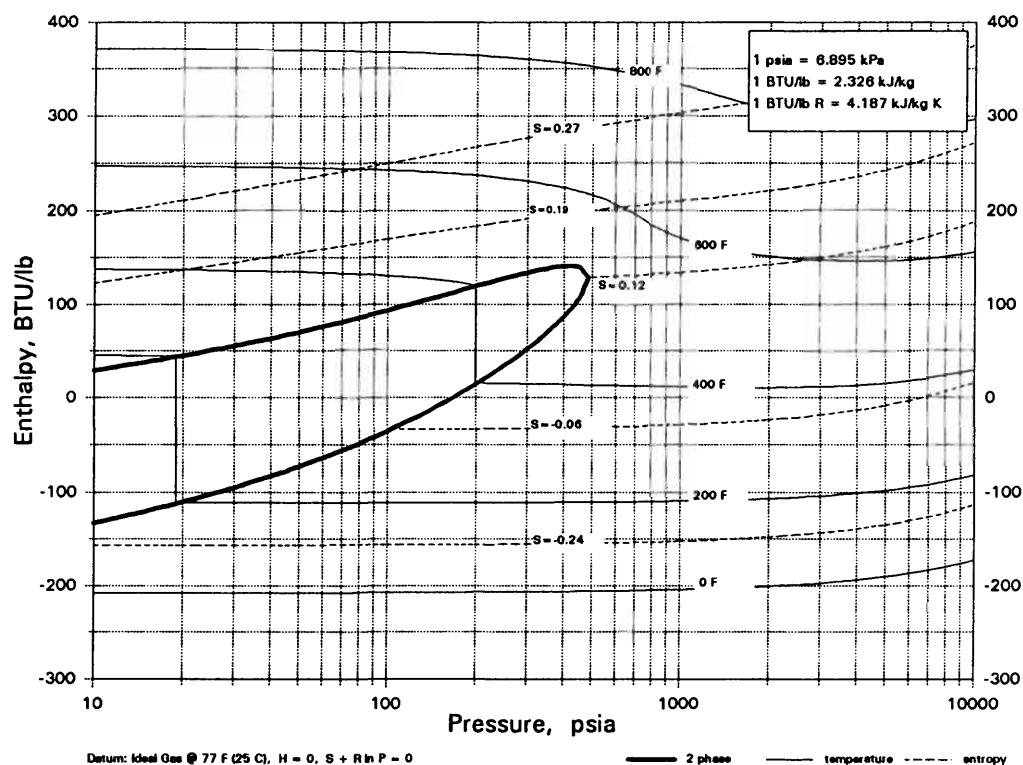
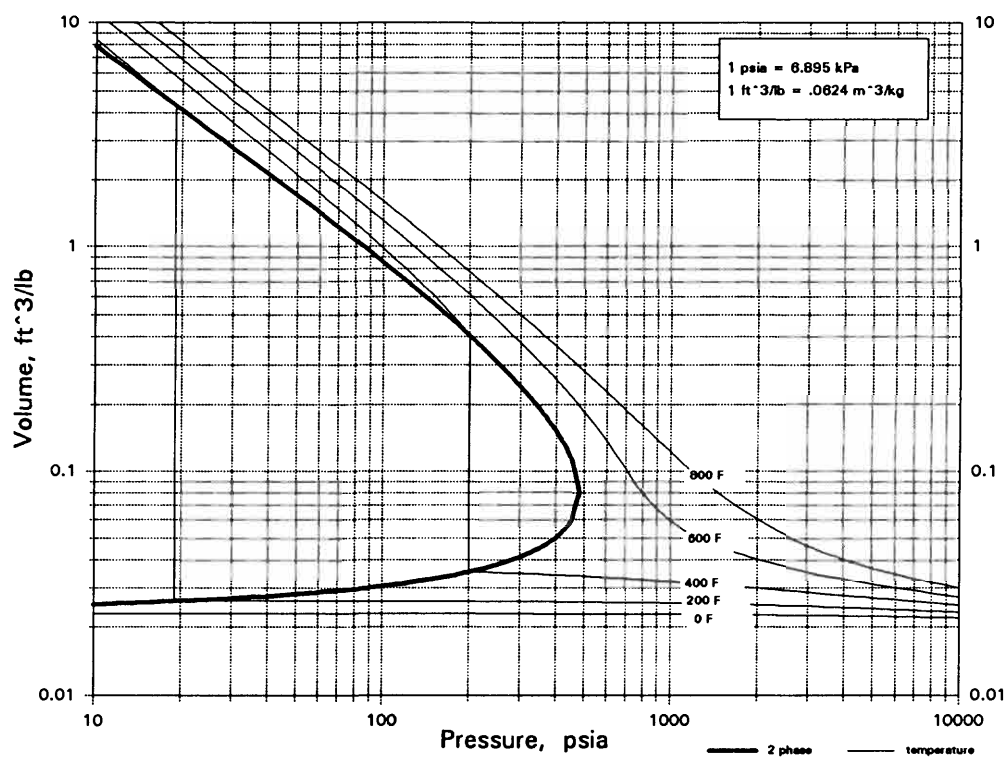
C6H10

1-5-HEXADIENE



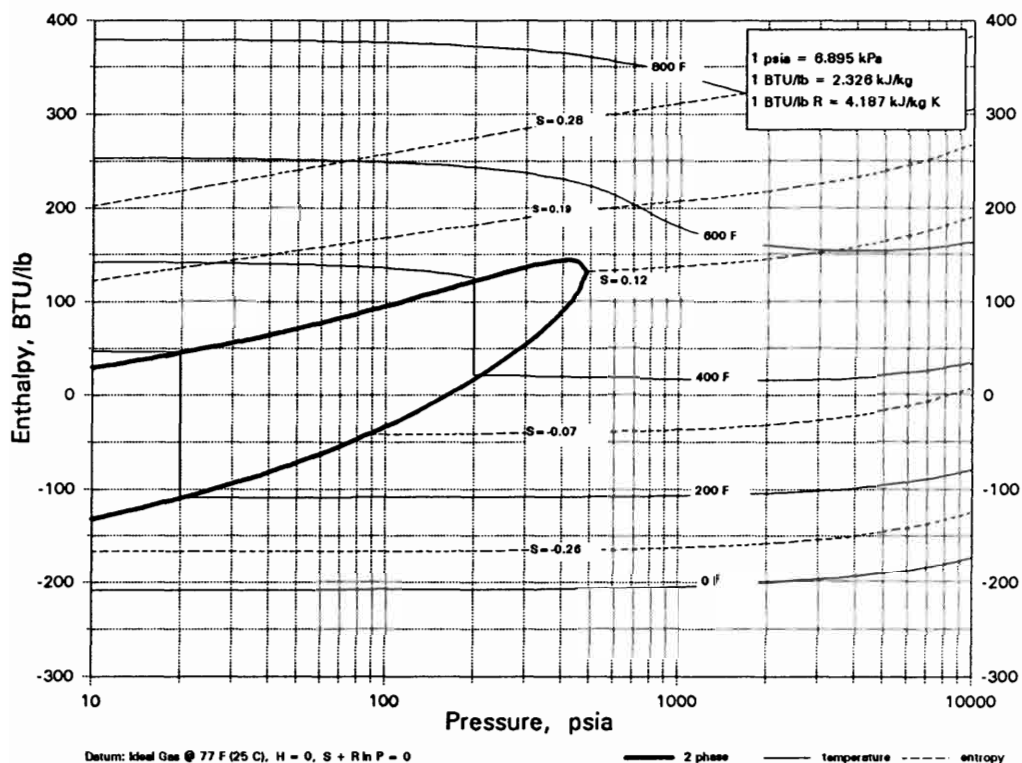
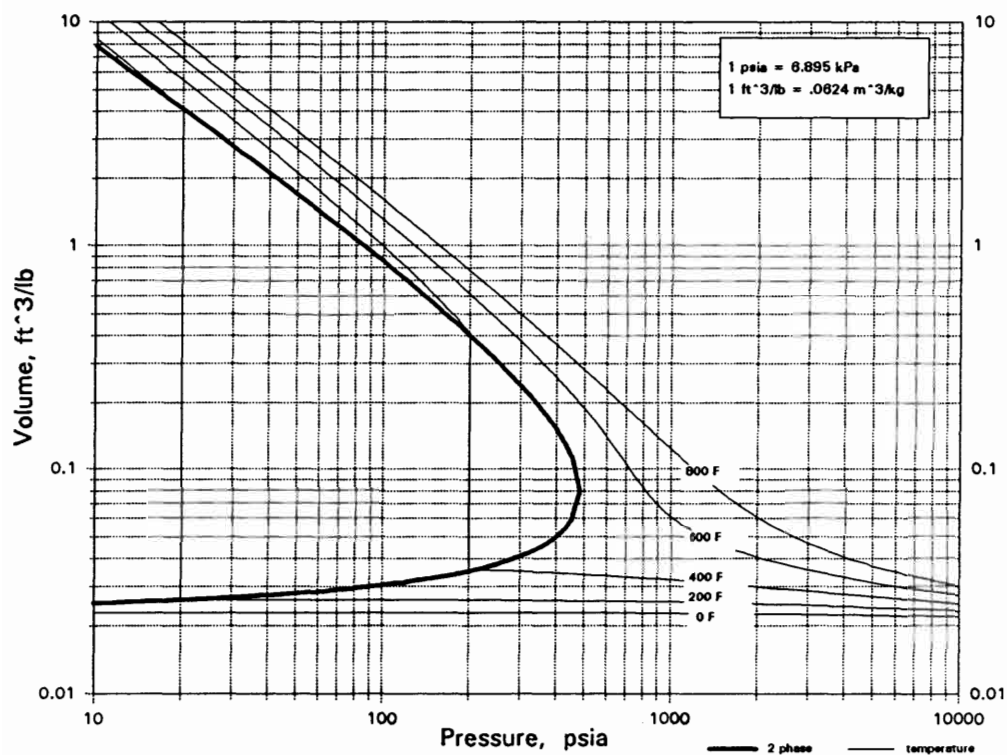
C6H10

cis-trans-2-4-HEXADIENE



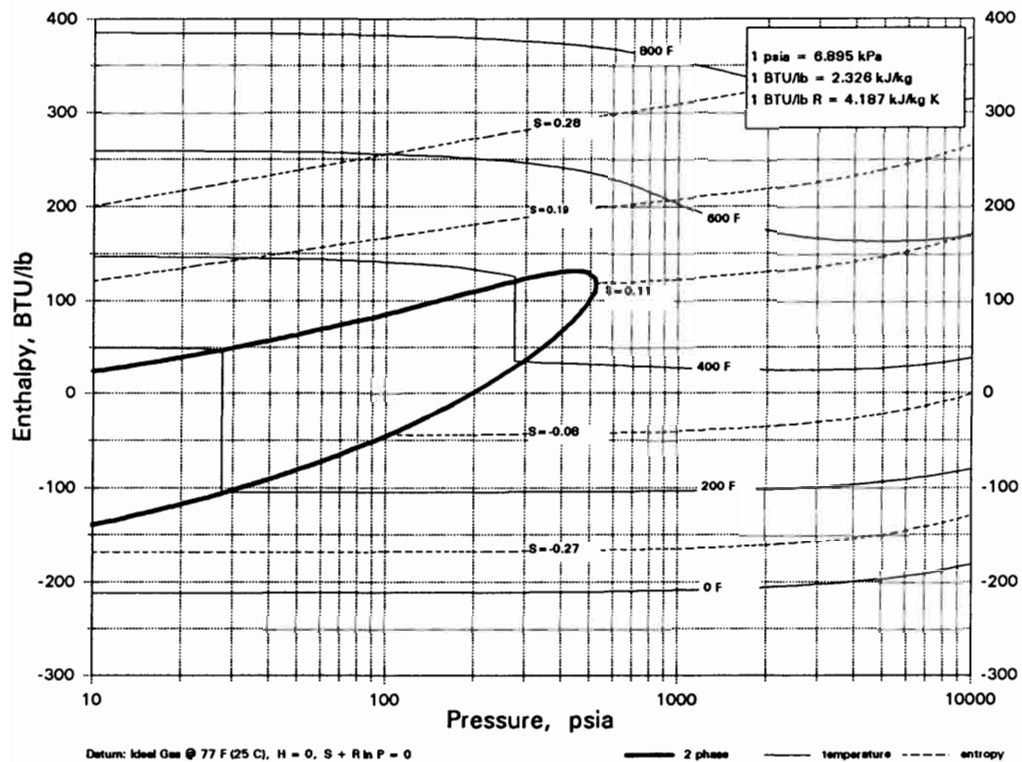
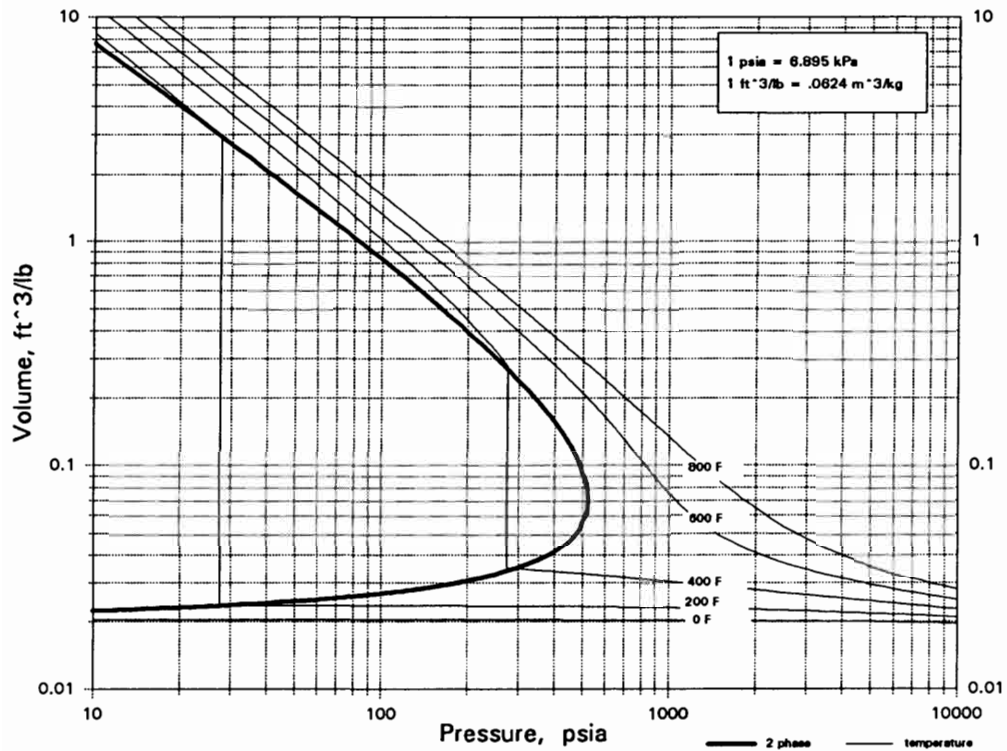
C6H10

trans-trans-2-4-HEXADIENE



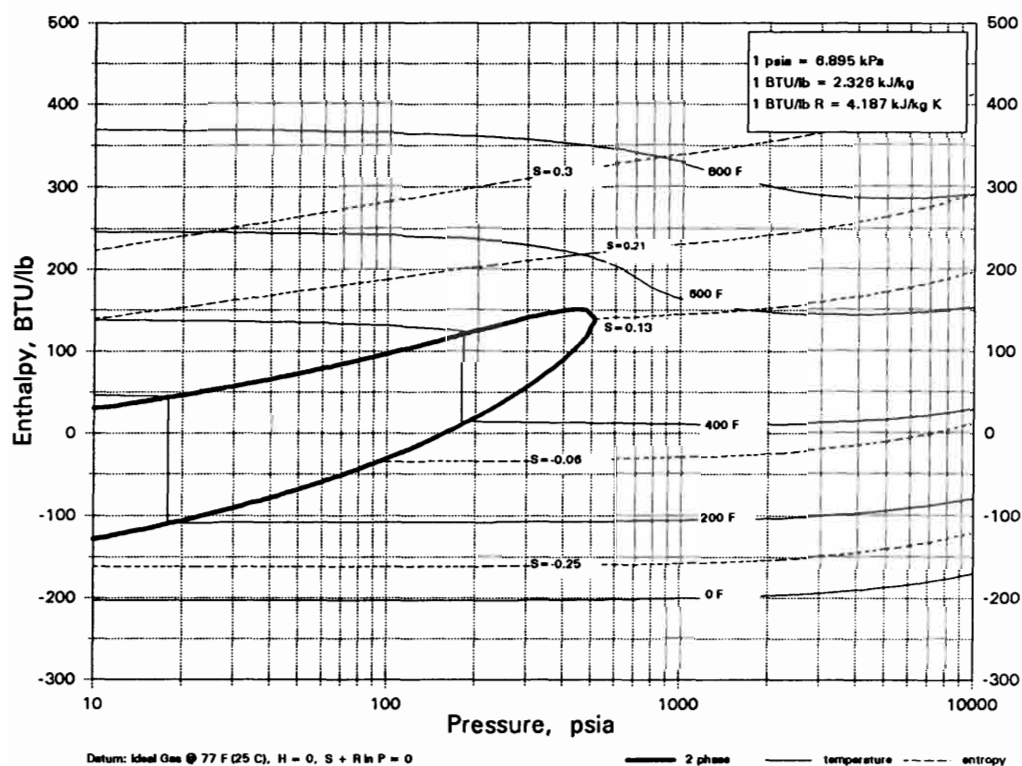
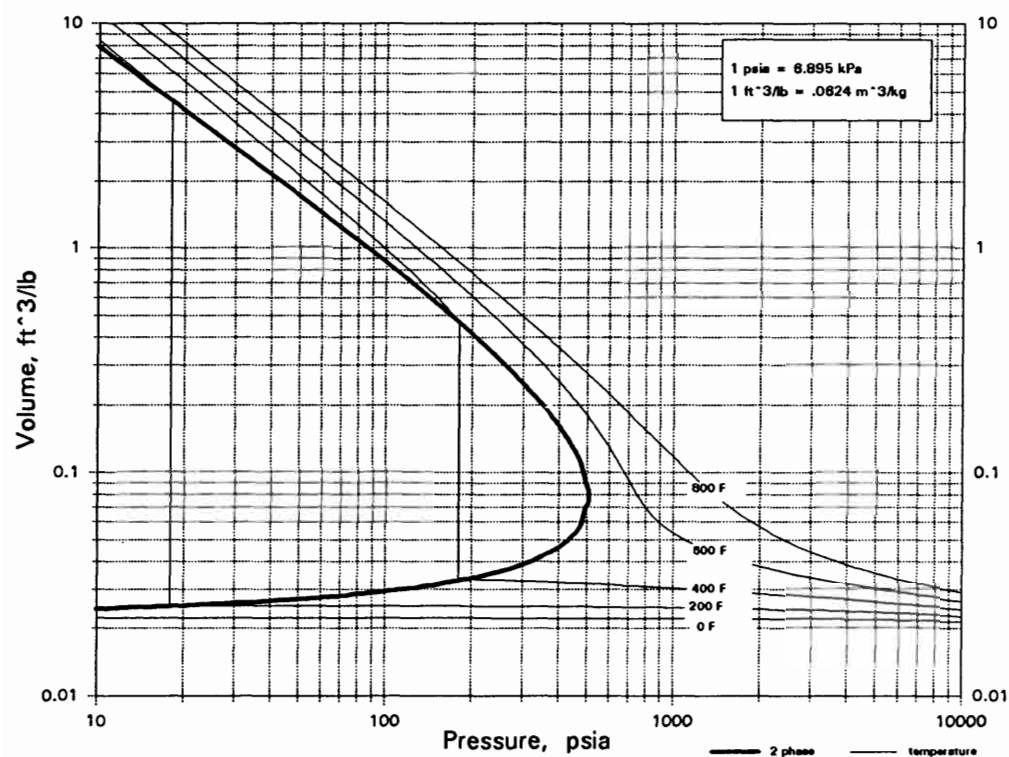
C6H10

1-HEXYNE



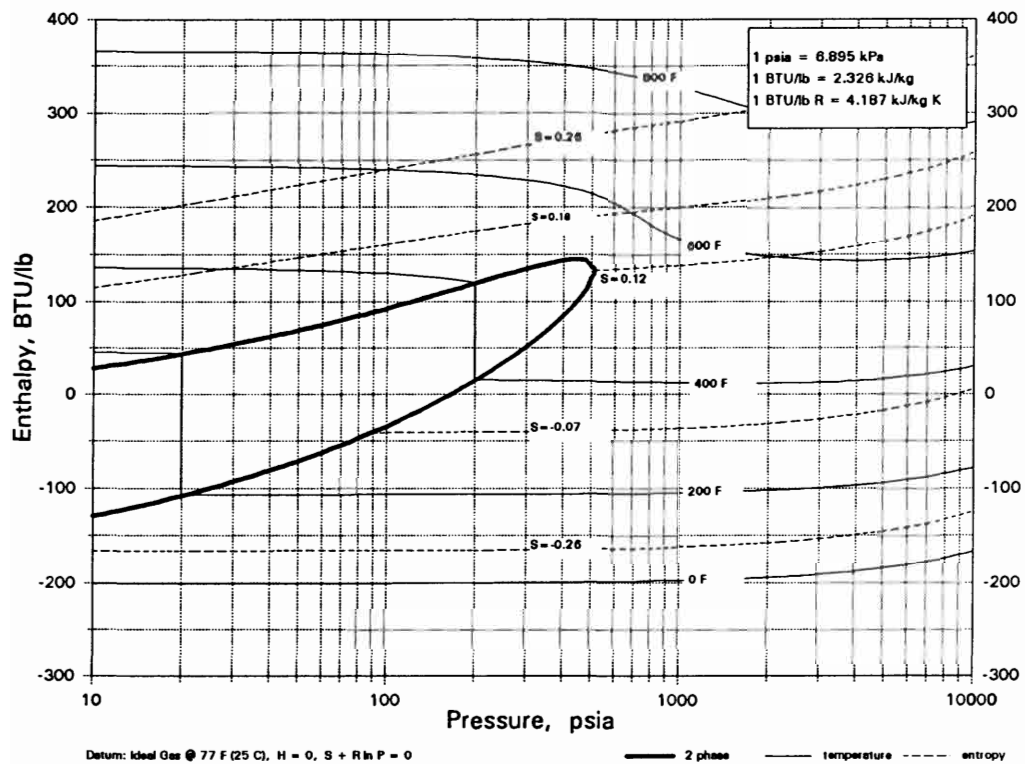
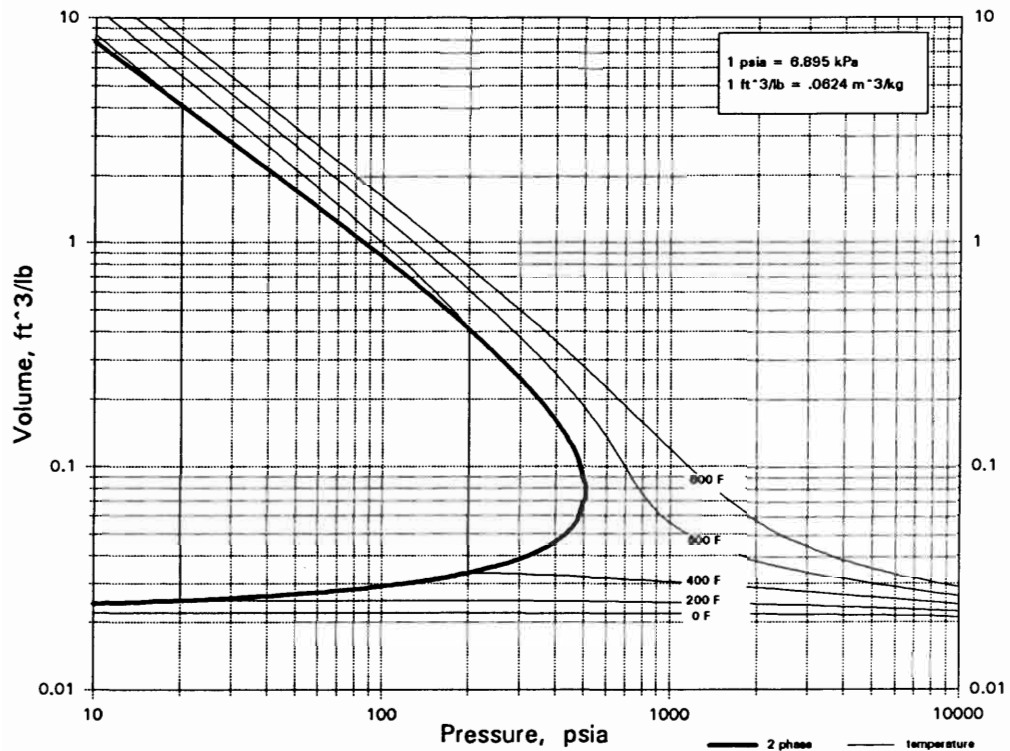
C6H10

2-HEXYNE



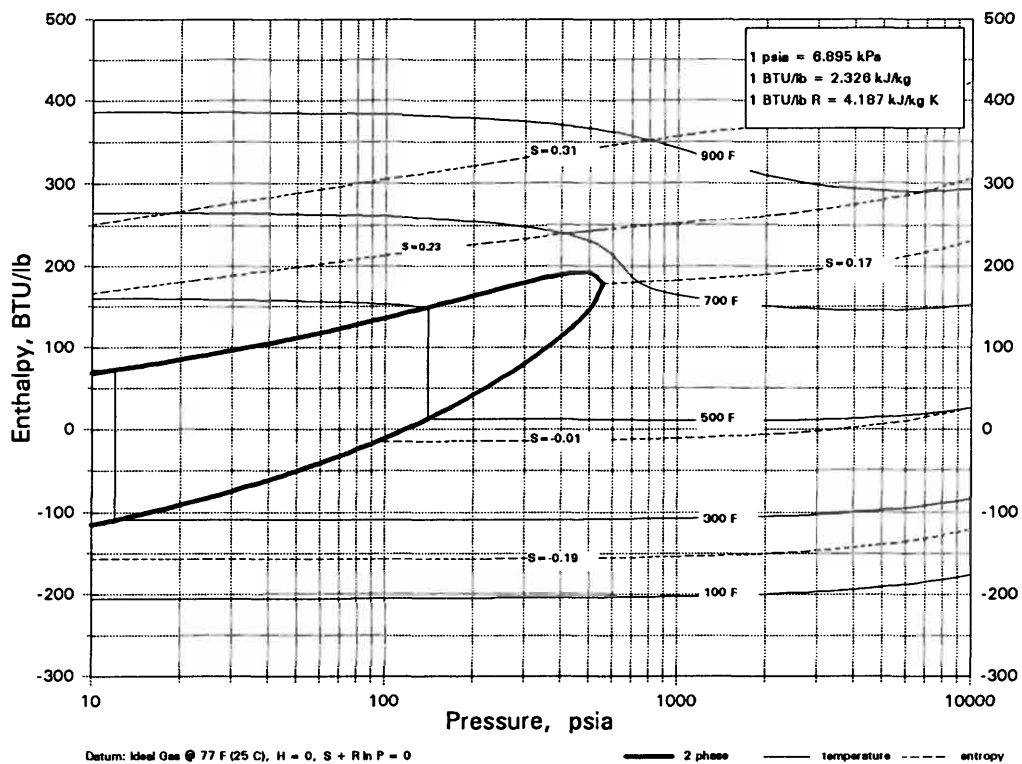
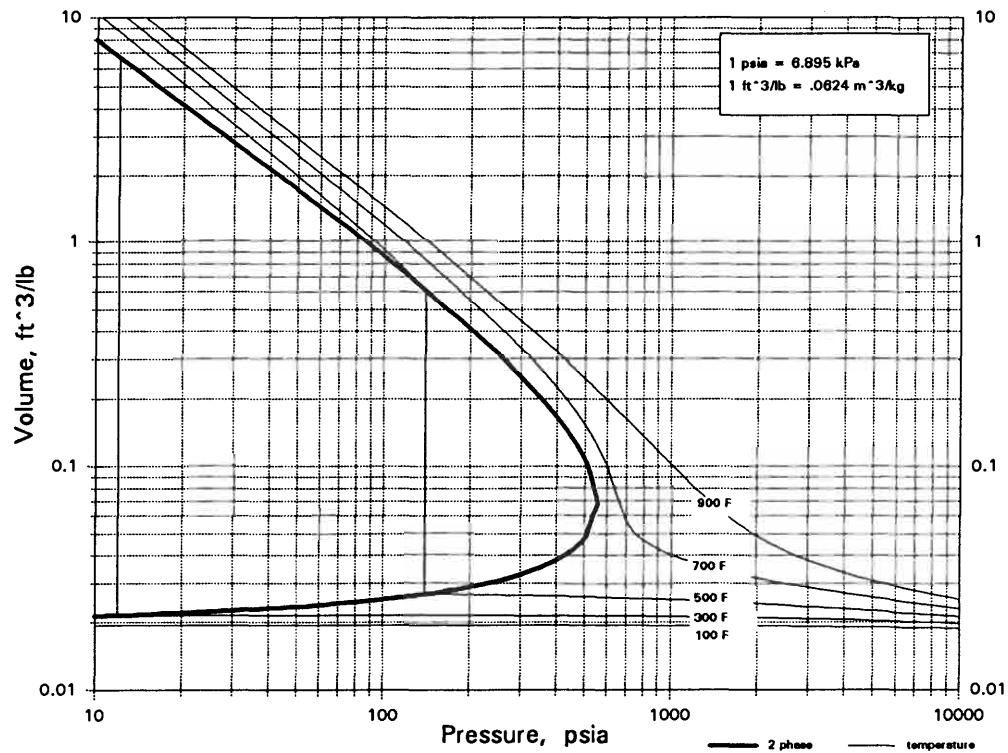
C6H10

3-HEXYNE



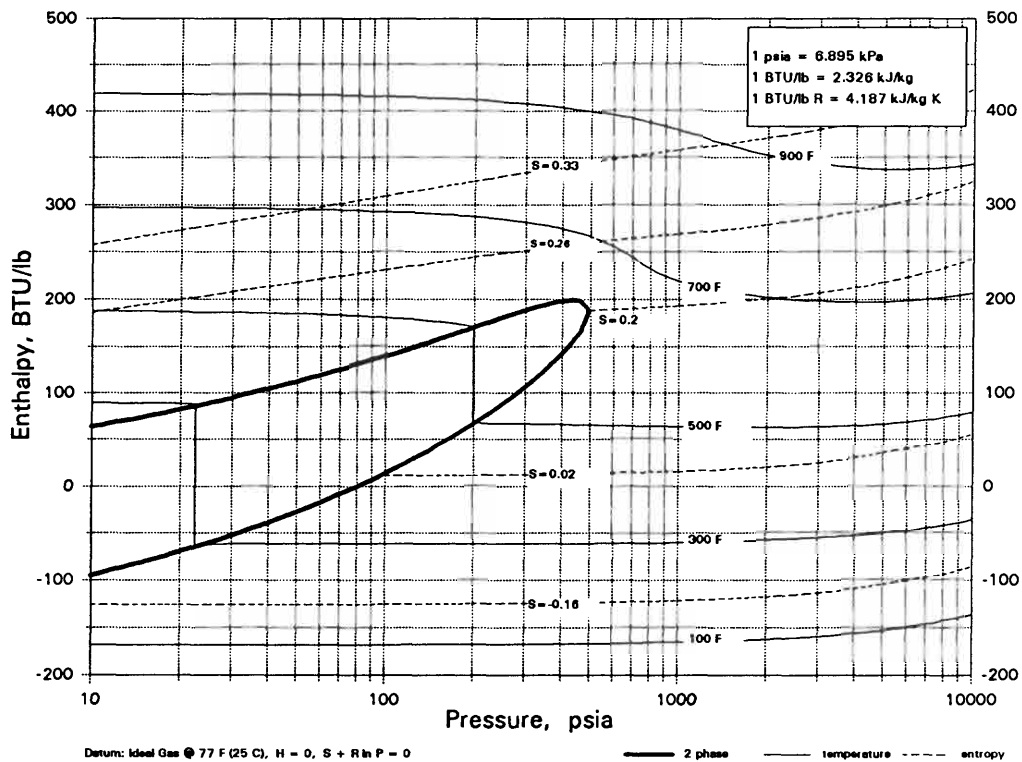
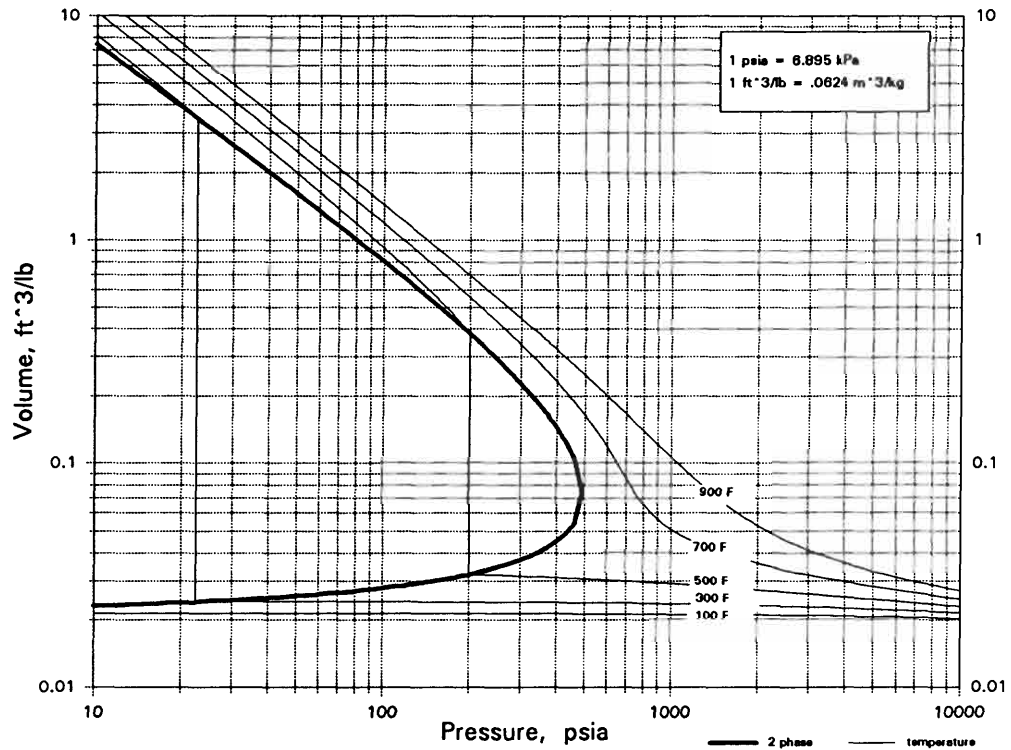
C6H10O

CYCLOHEXANONE



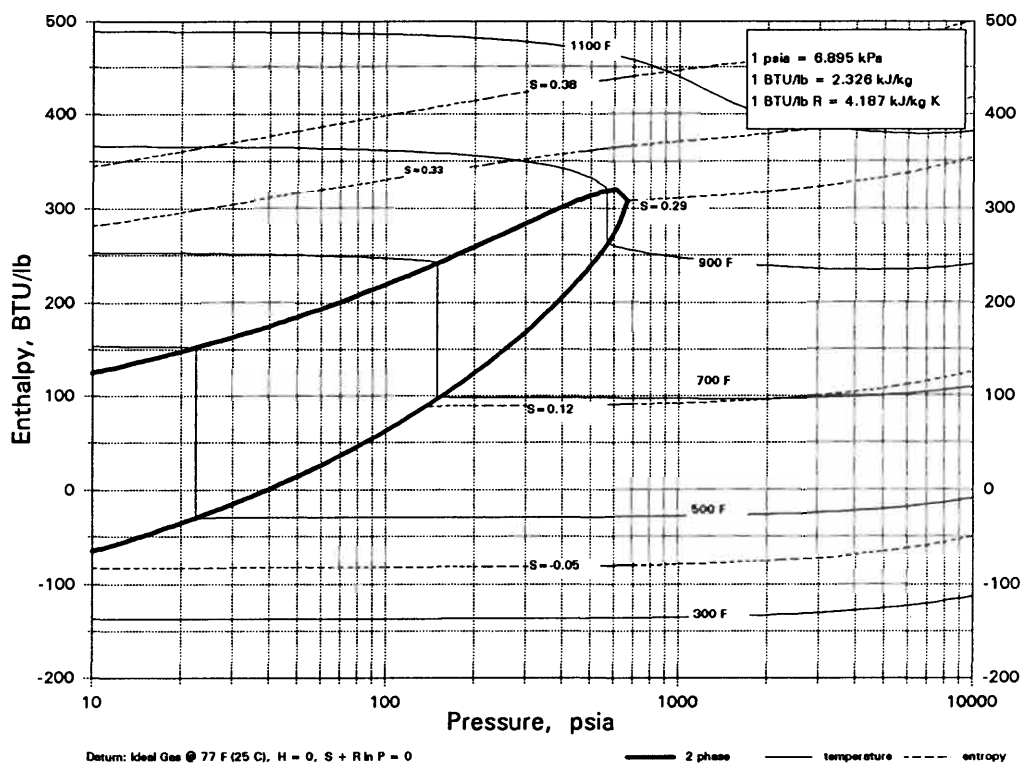
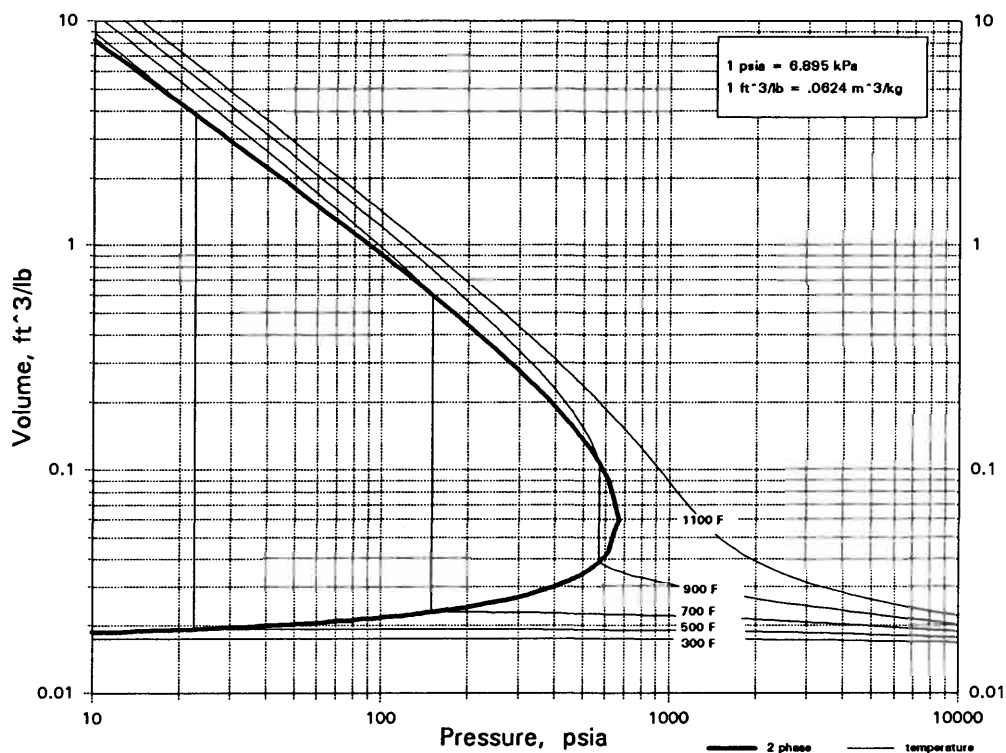
C6H10O

MESITYL OXIDE



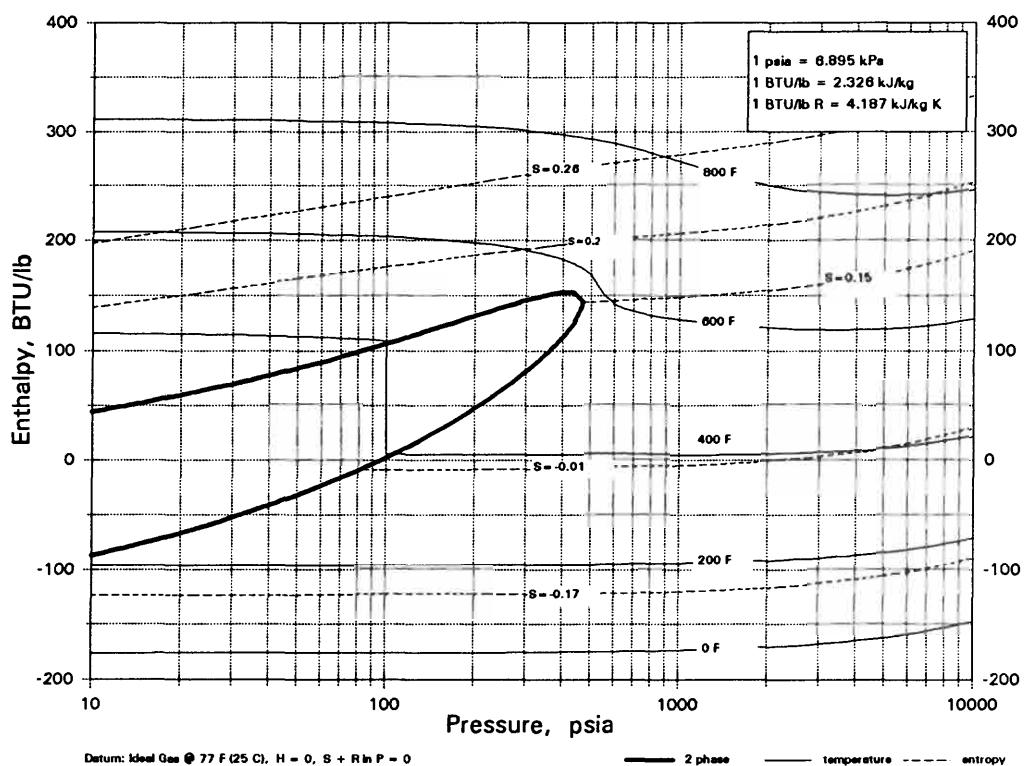
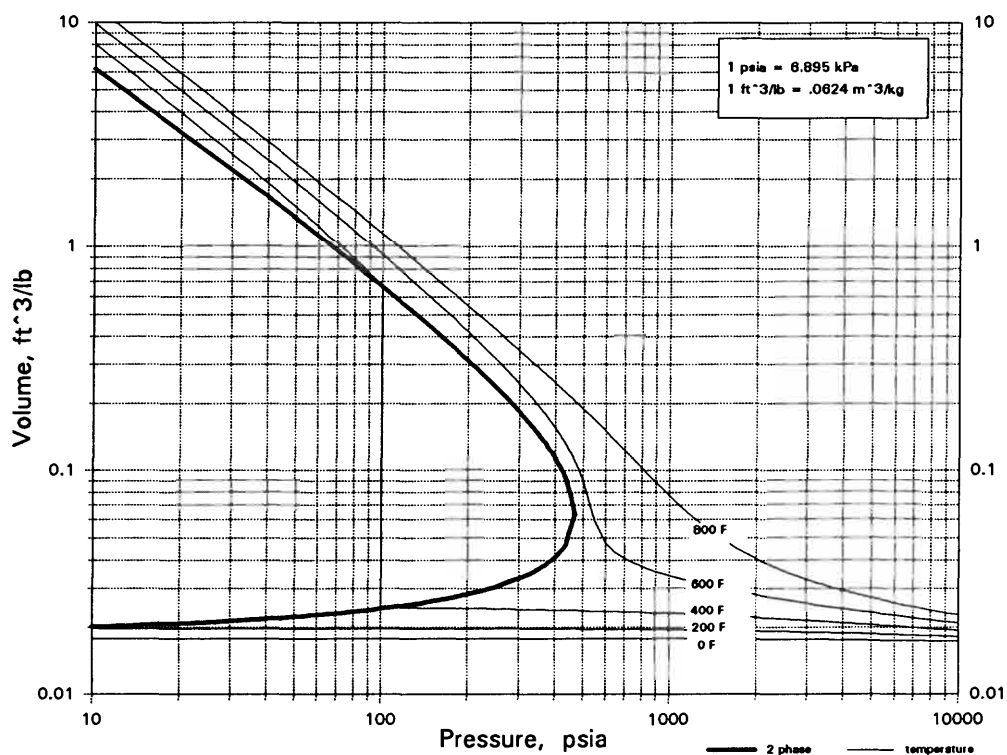
C6H10O2

epsilon-CAPROLACTONE



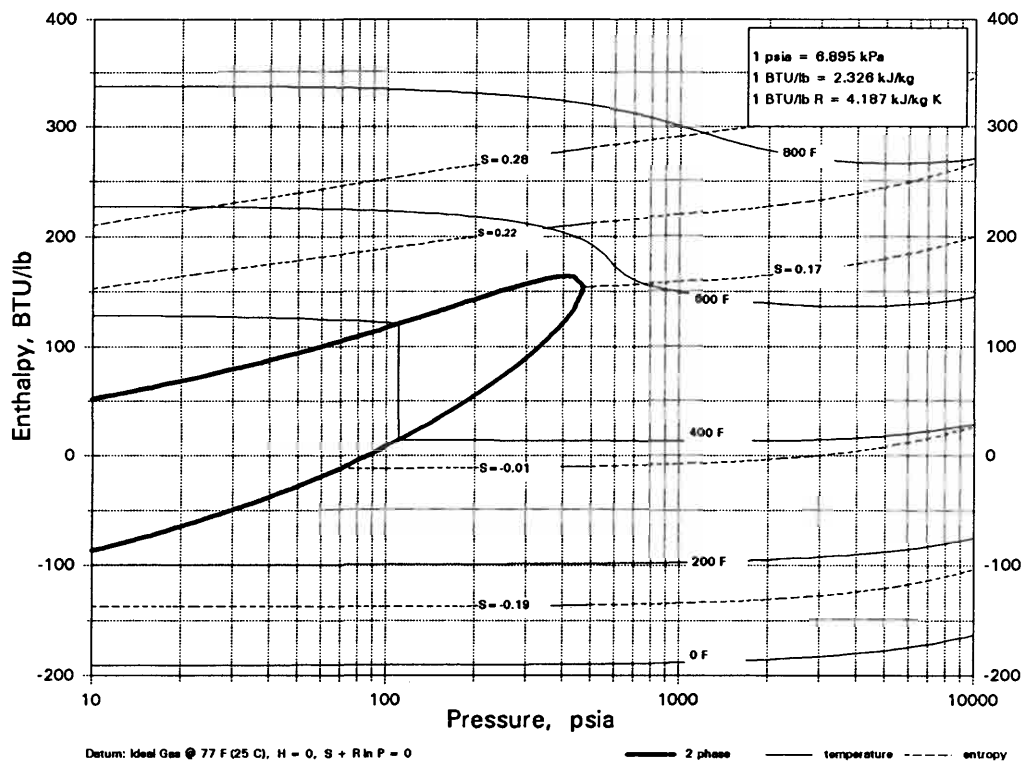
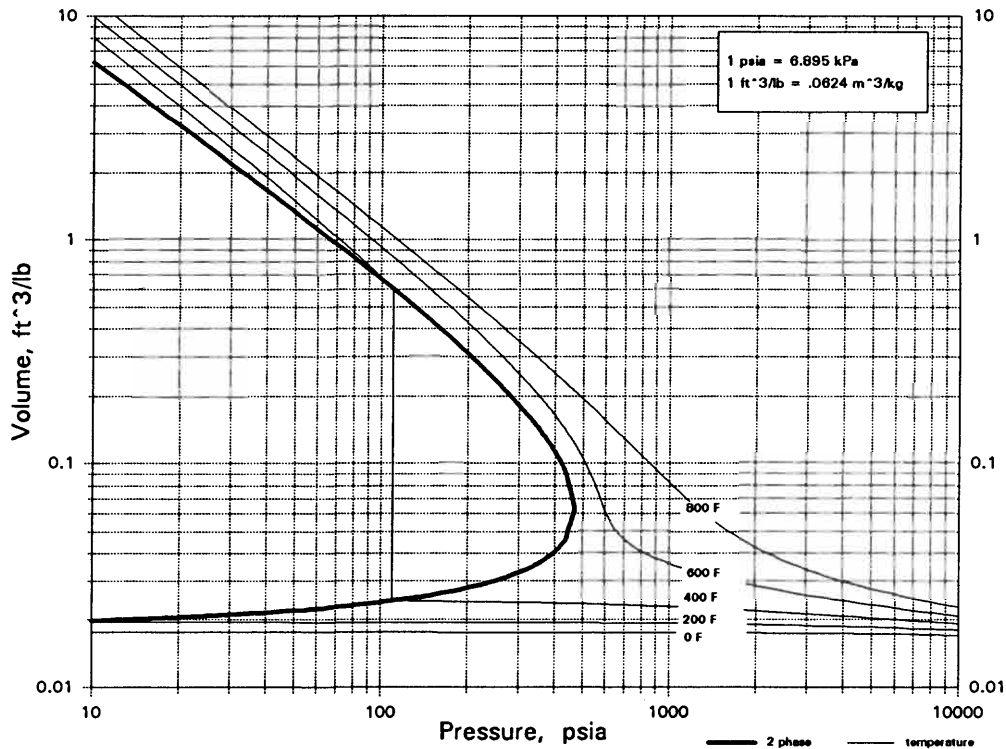
C6H10O2

ETHYL METHACRYLATE



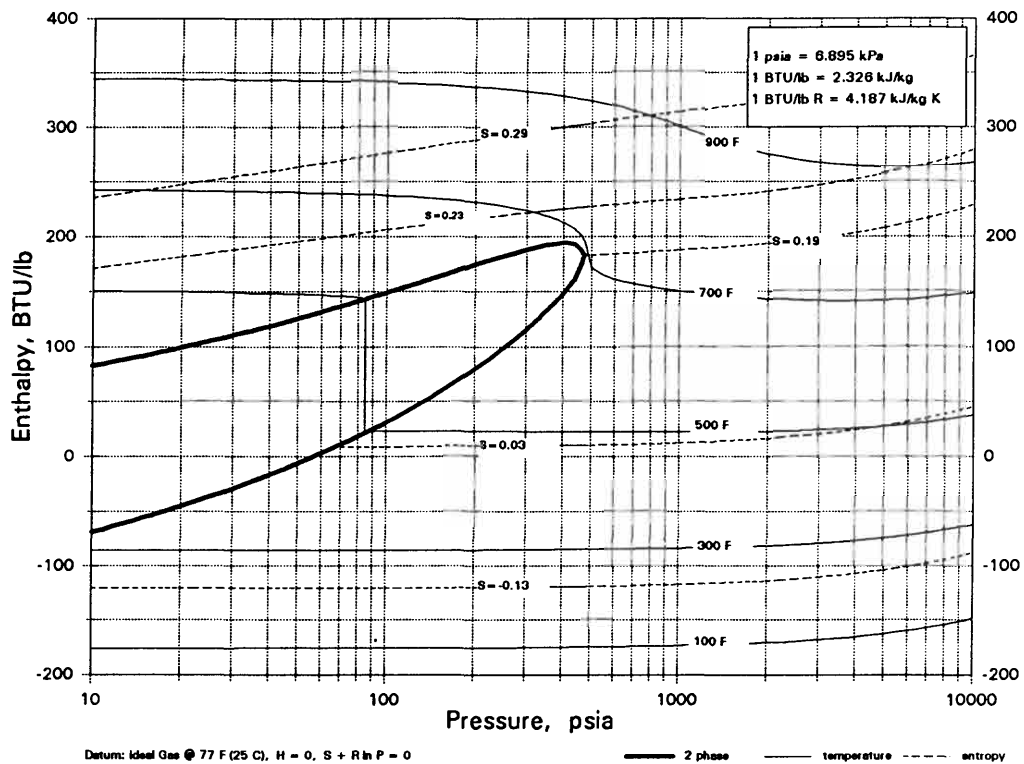
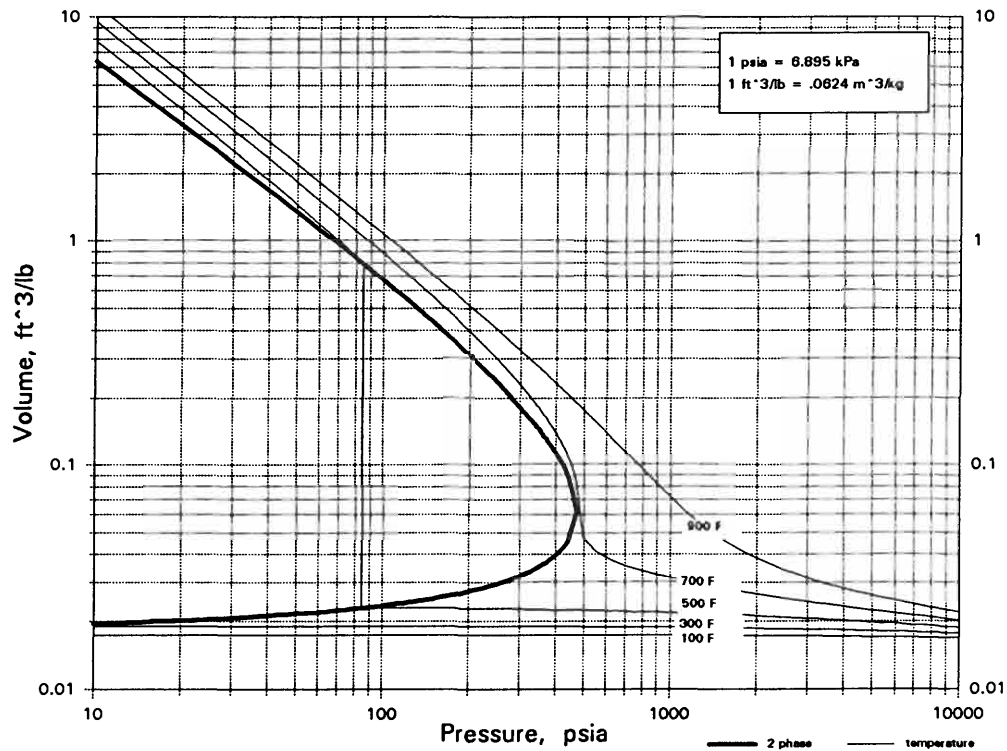
C6H10O2

n-PROPYL ACRYLATE



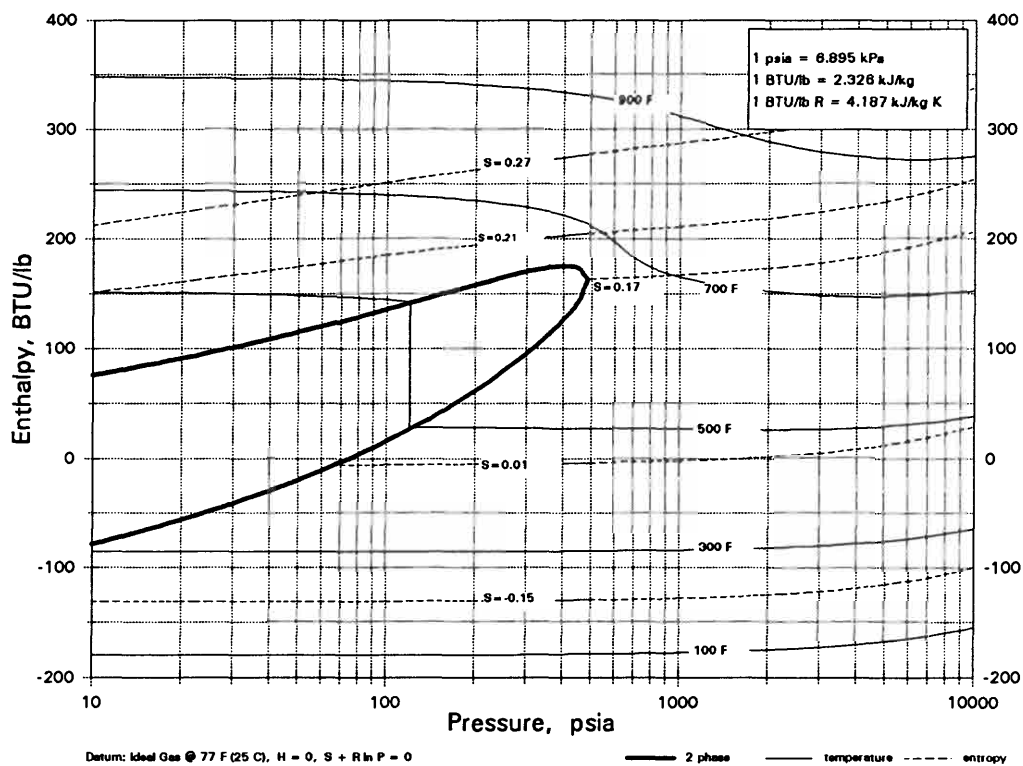
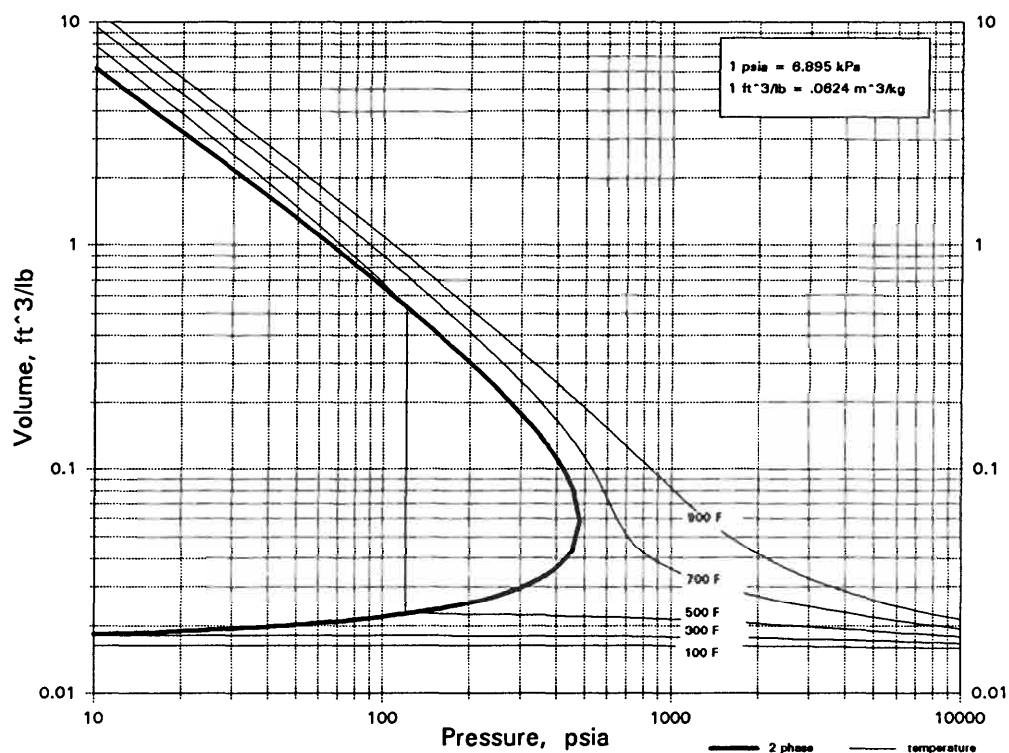
C6H10O3

ETHYLACETOACETATE



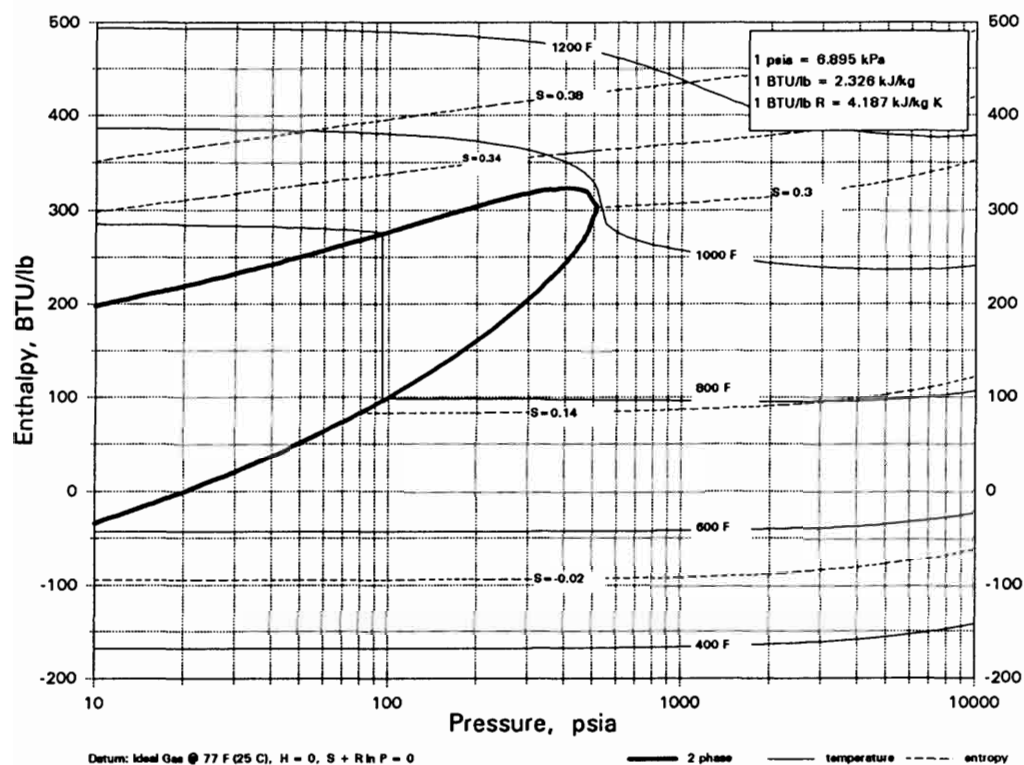
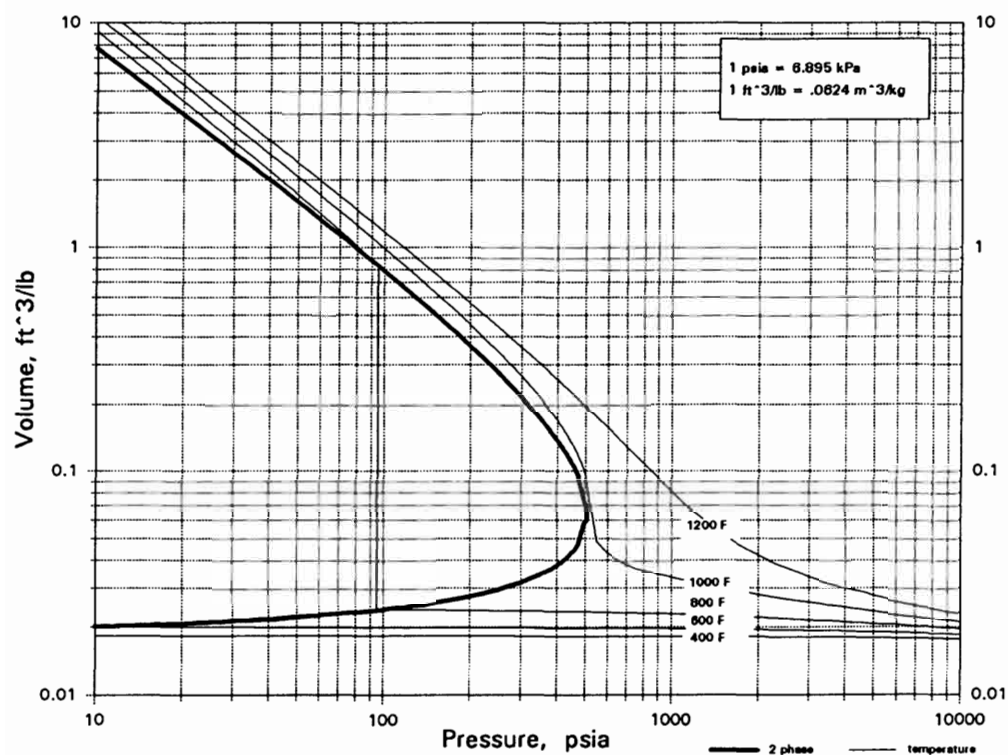
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PROPIONIC ANHYDRIDE



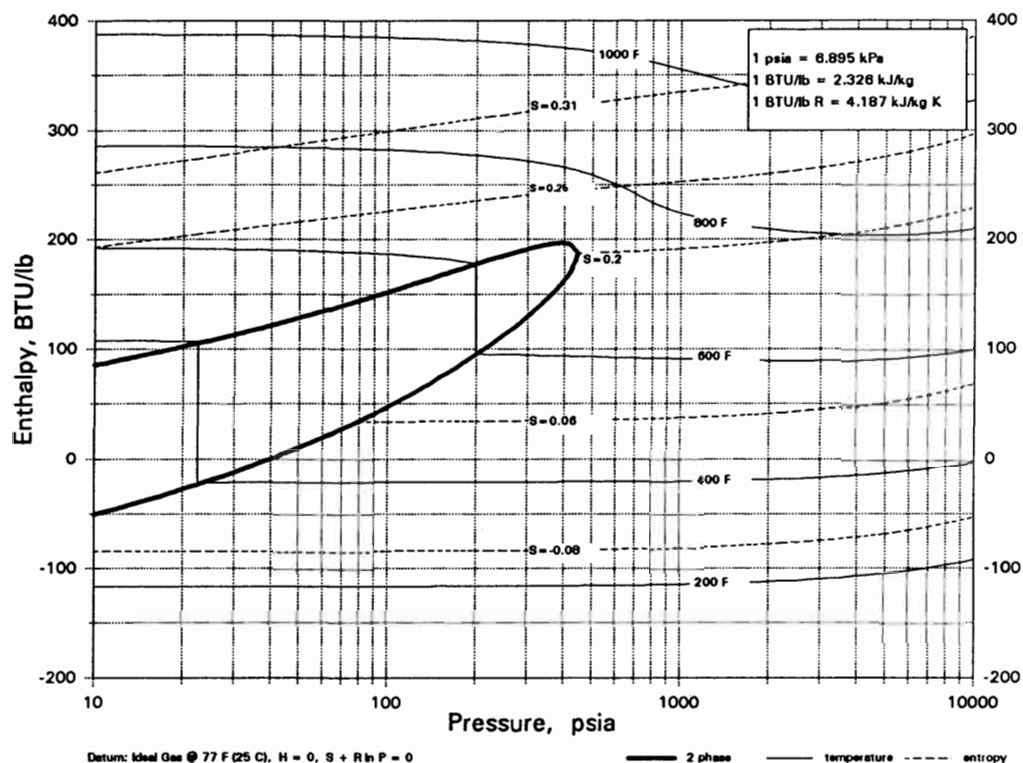
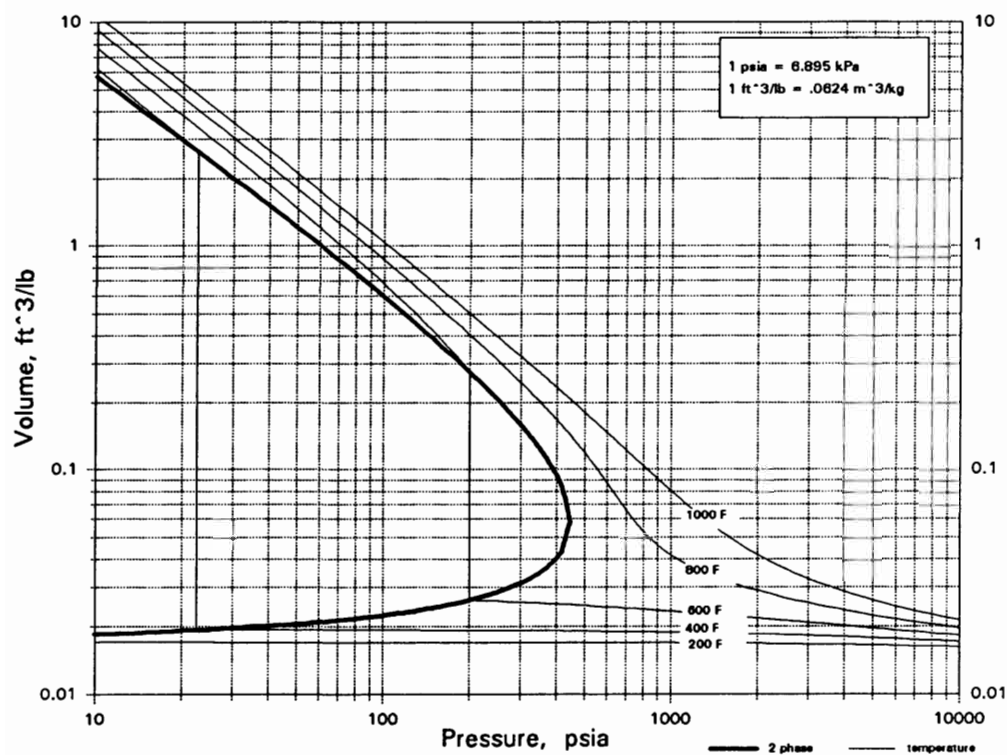
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ADIPIC ACID



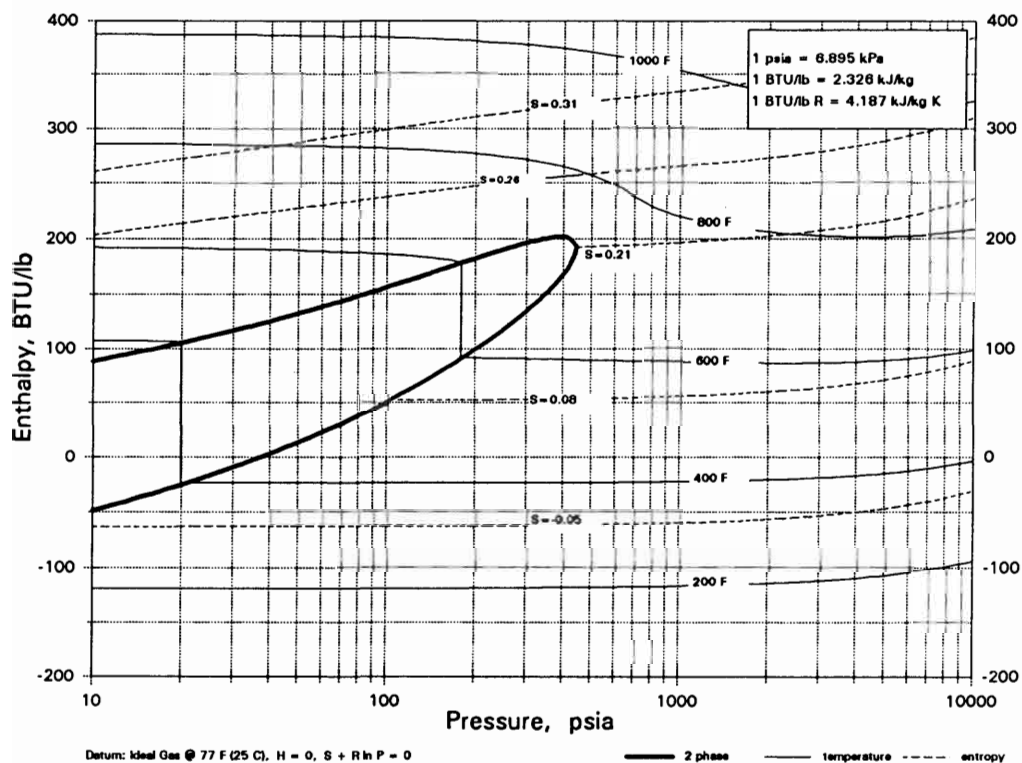
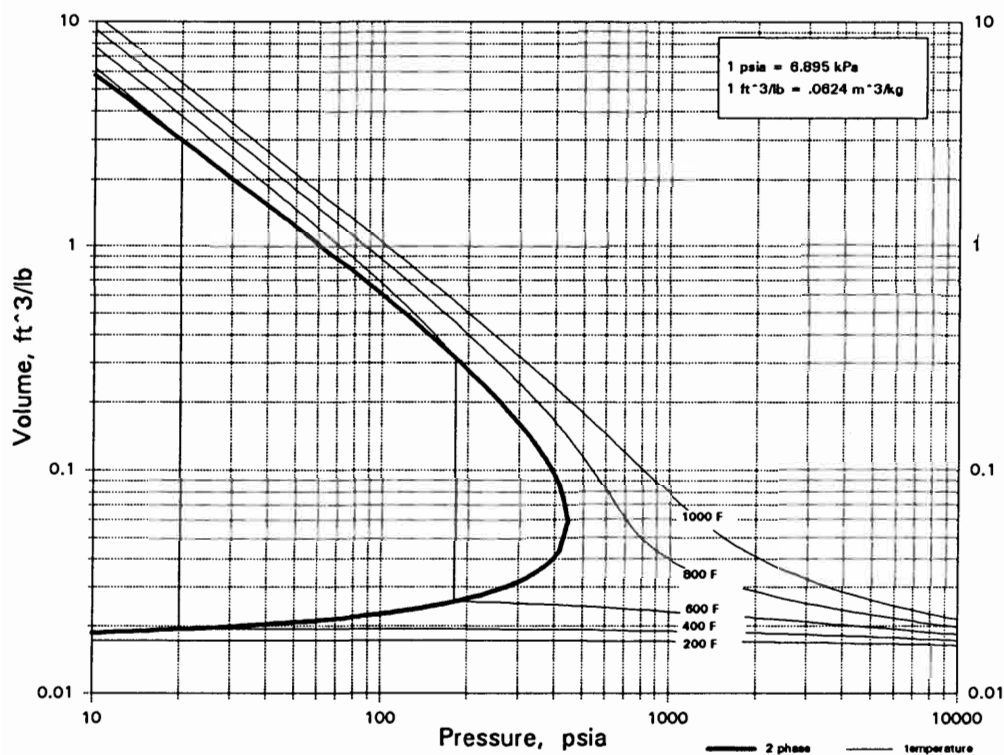
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DIETHYL OXALATE



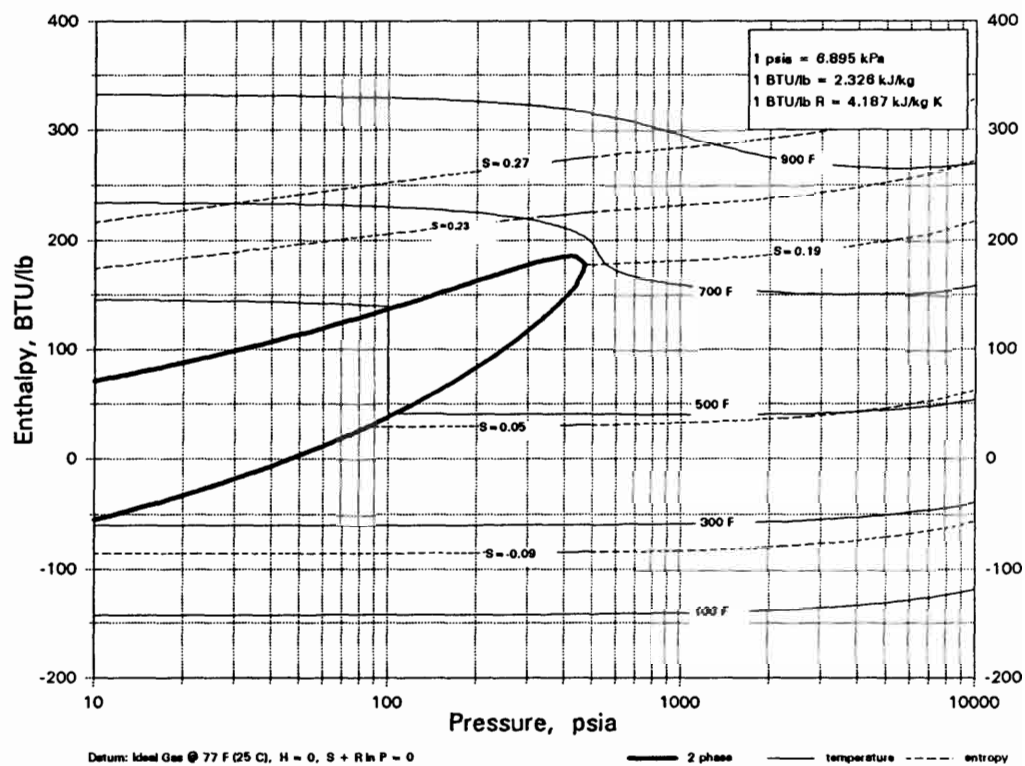
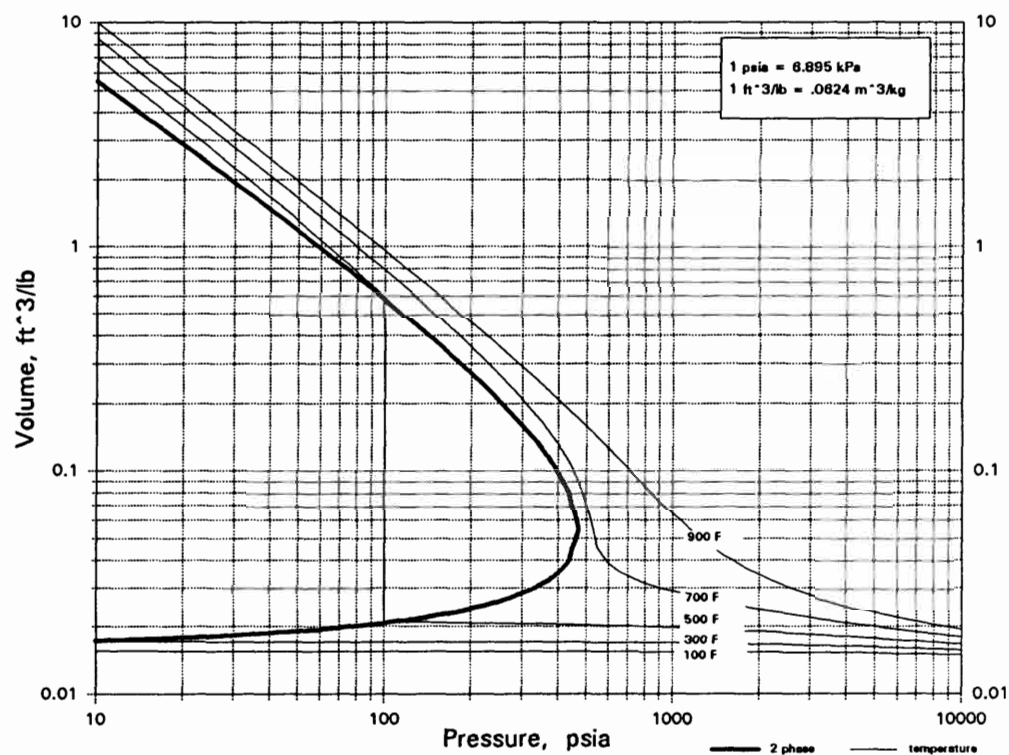
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ETHYLENE GLYCOL DIACETATE



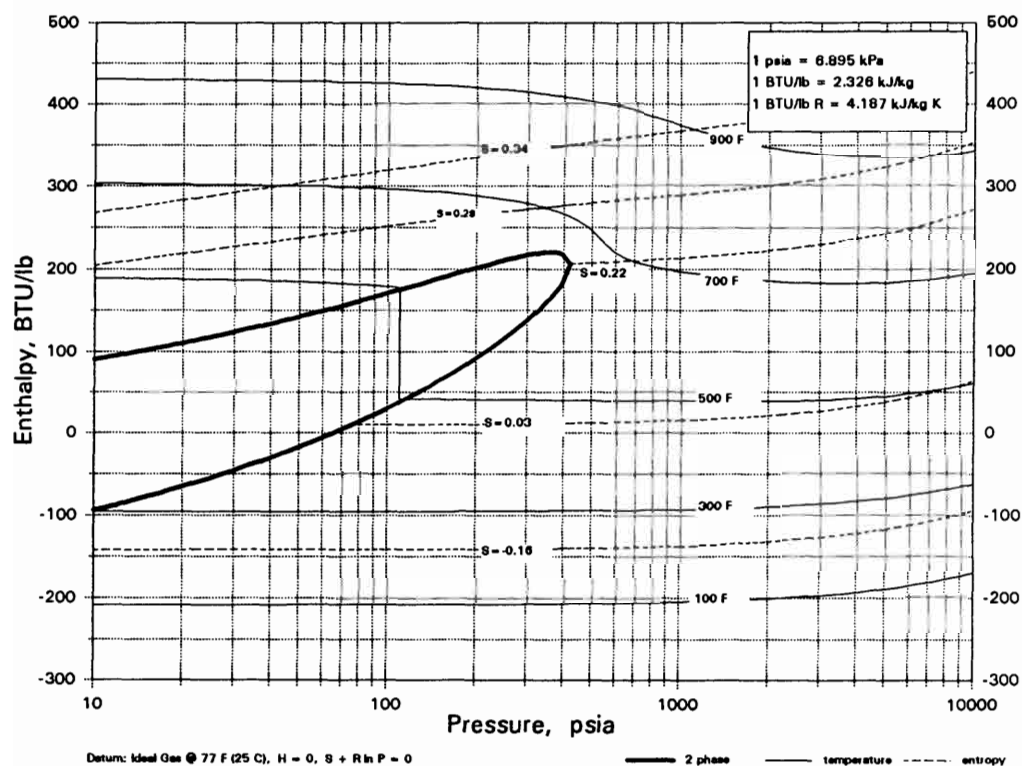
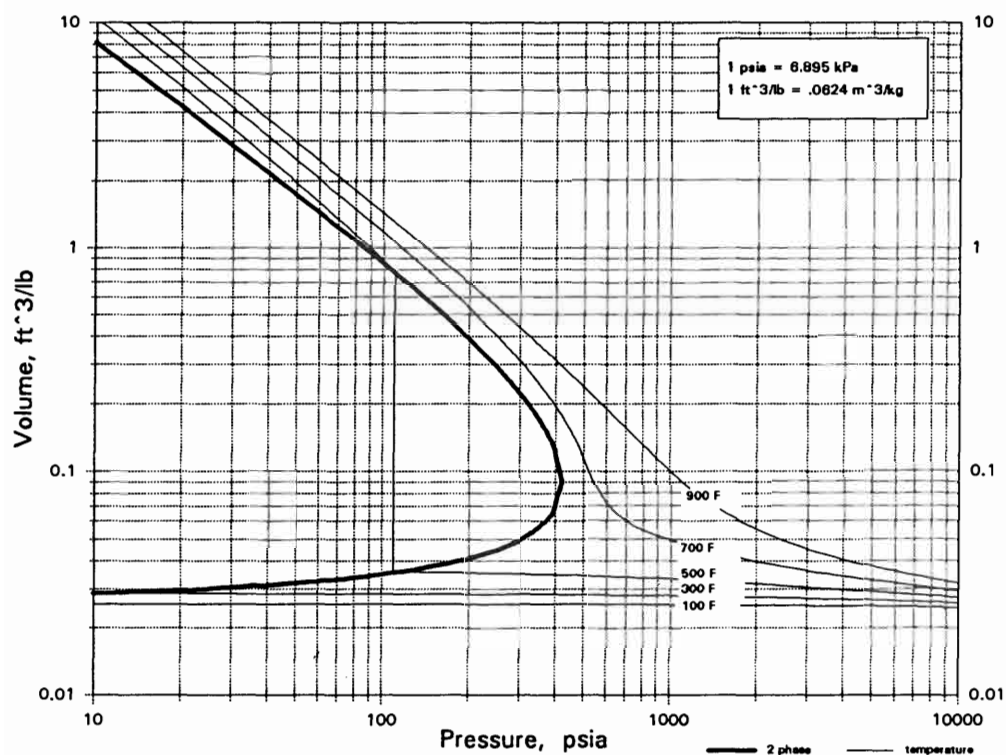
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ETHYLIDENE DIACETATE

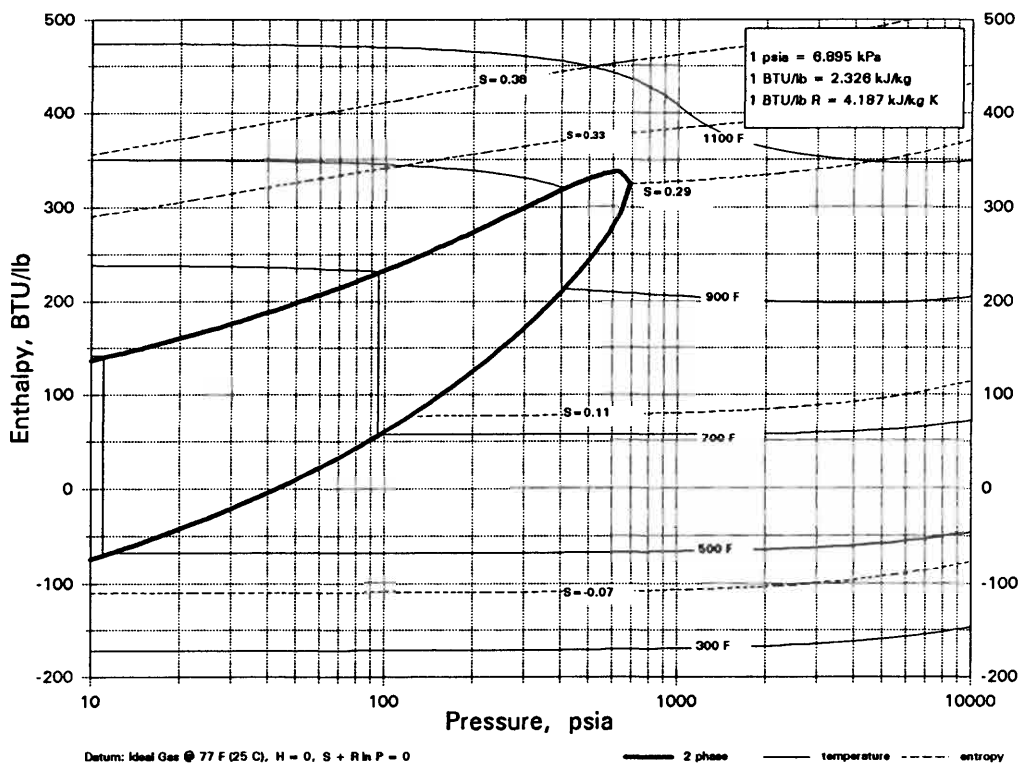
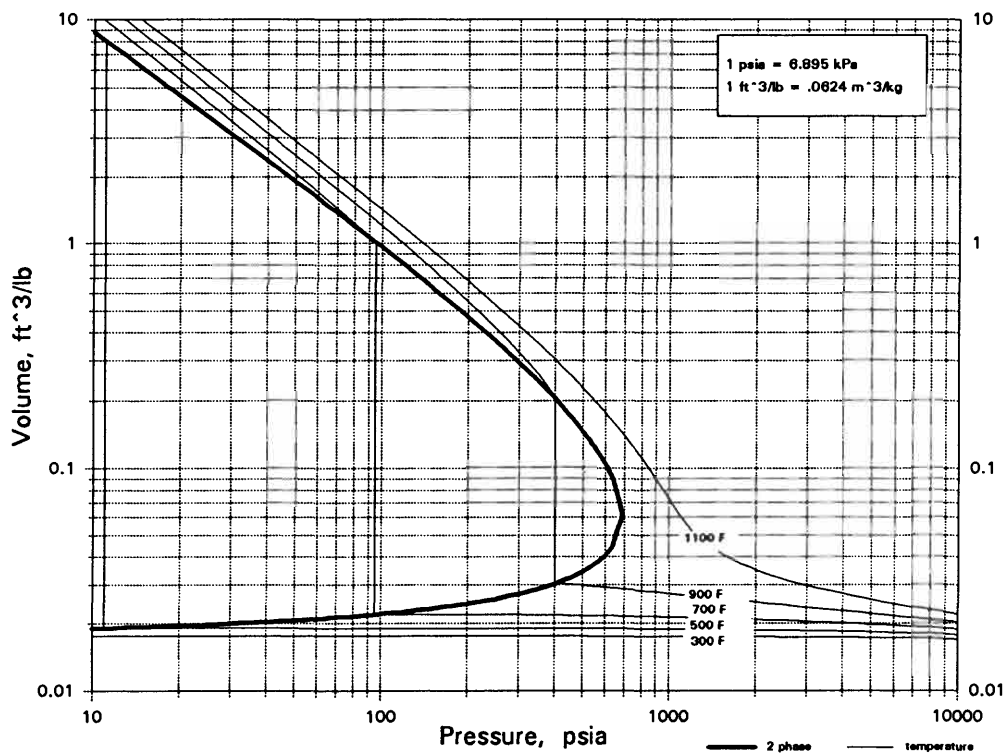


C6H11N

HEXANENITRILE

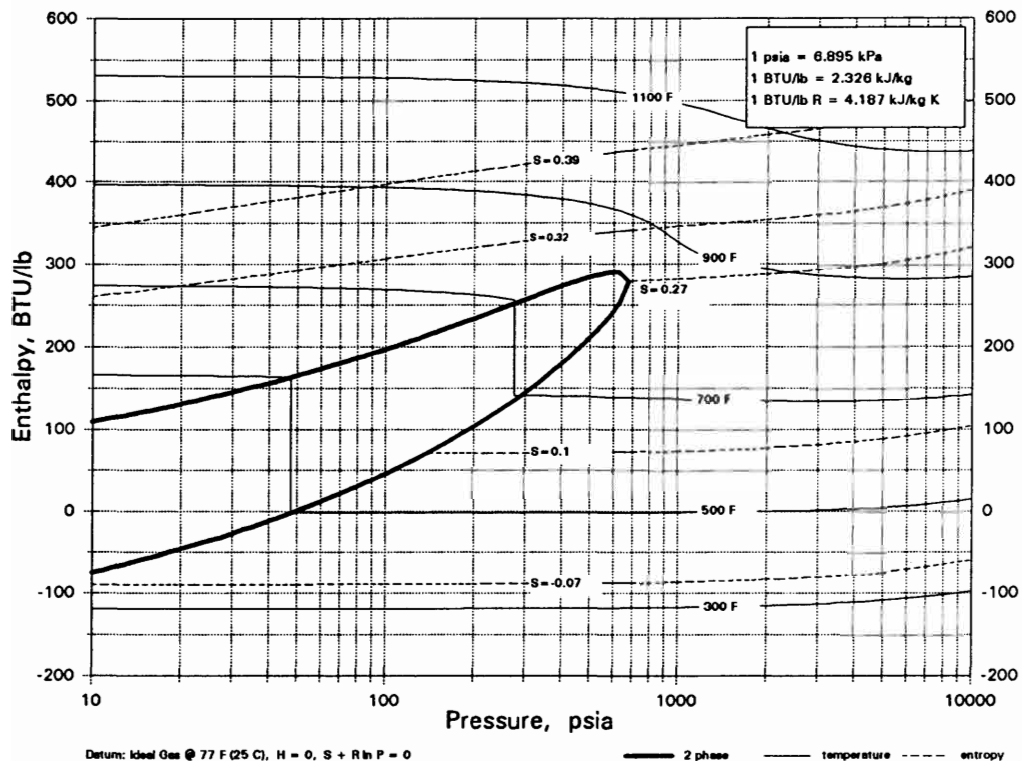
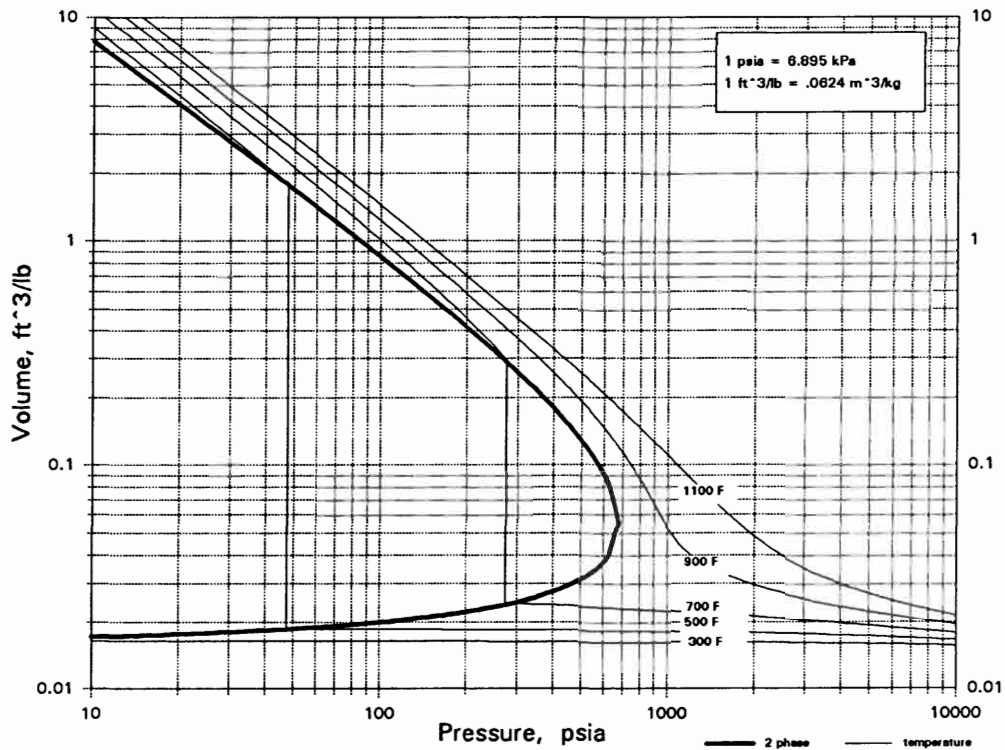


C6H11NO
epsilon-CAPROLACTAM



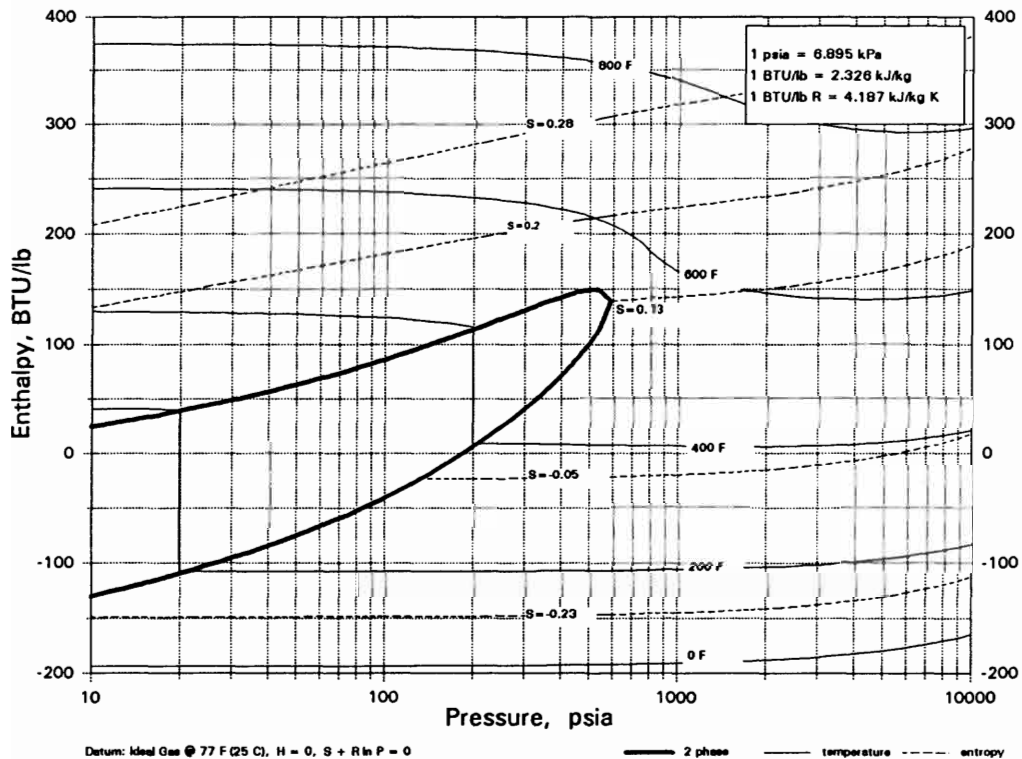
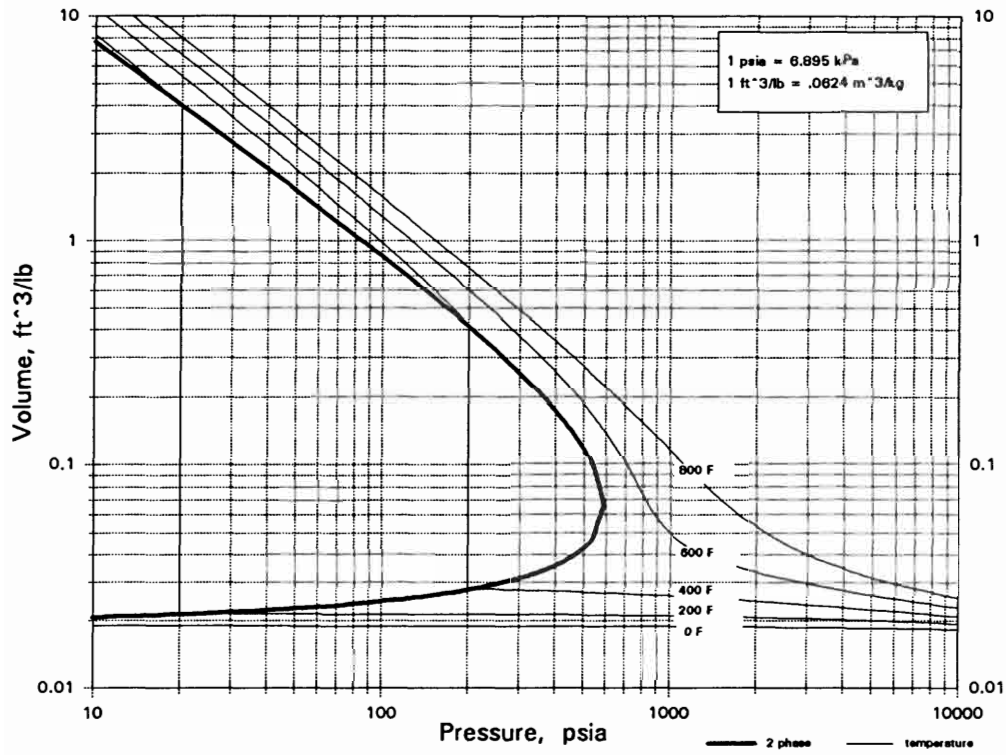
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CYCLOHEXANONE OXIME



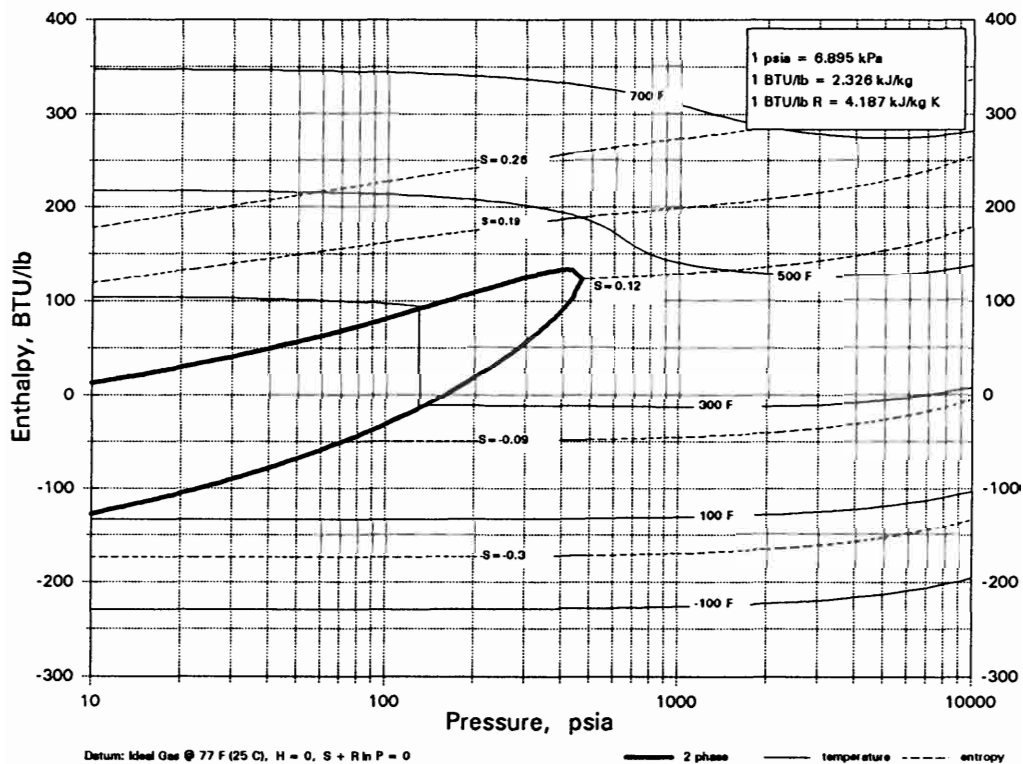
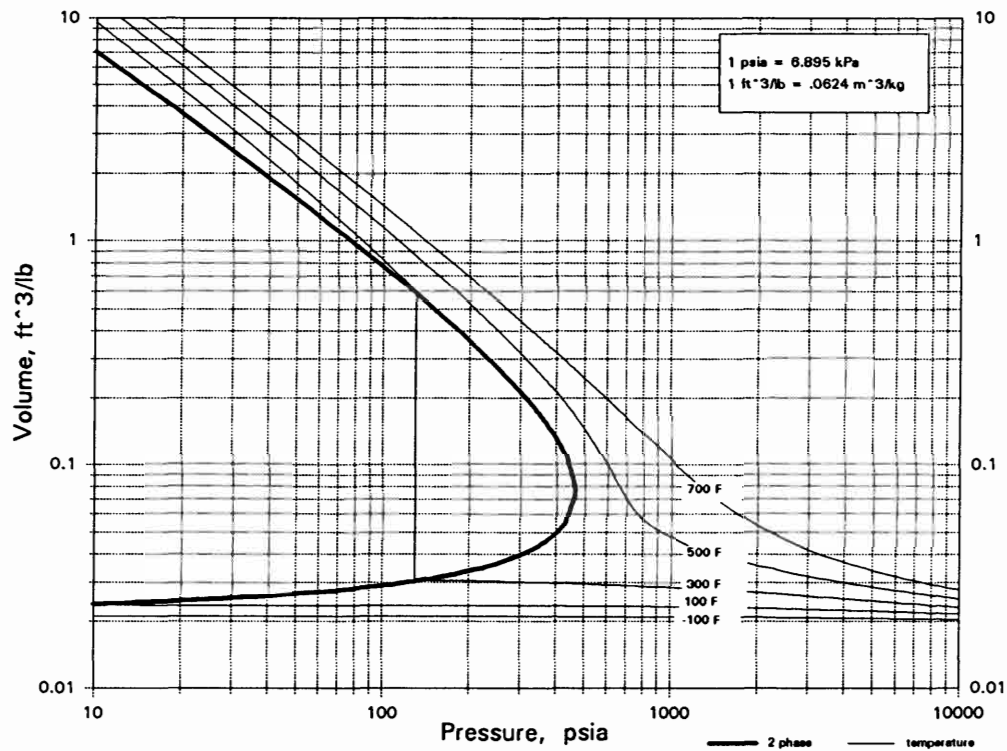
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CYCLOHEXANE



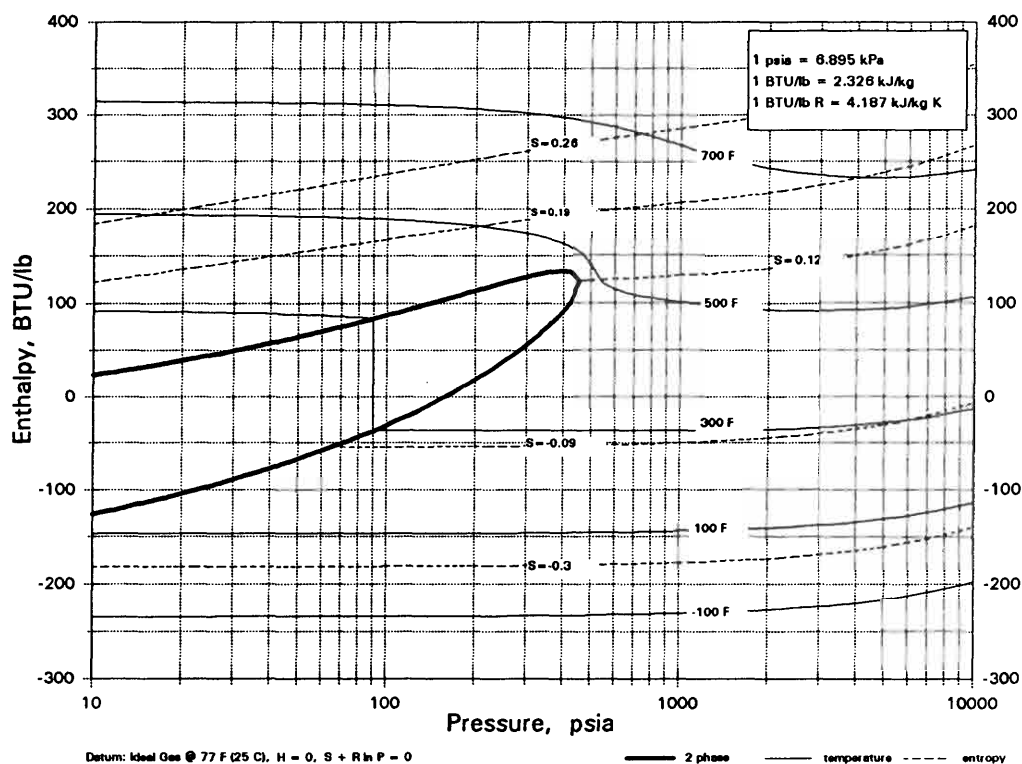
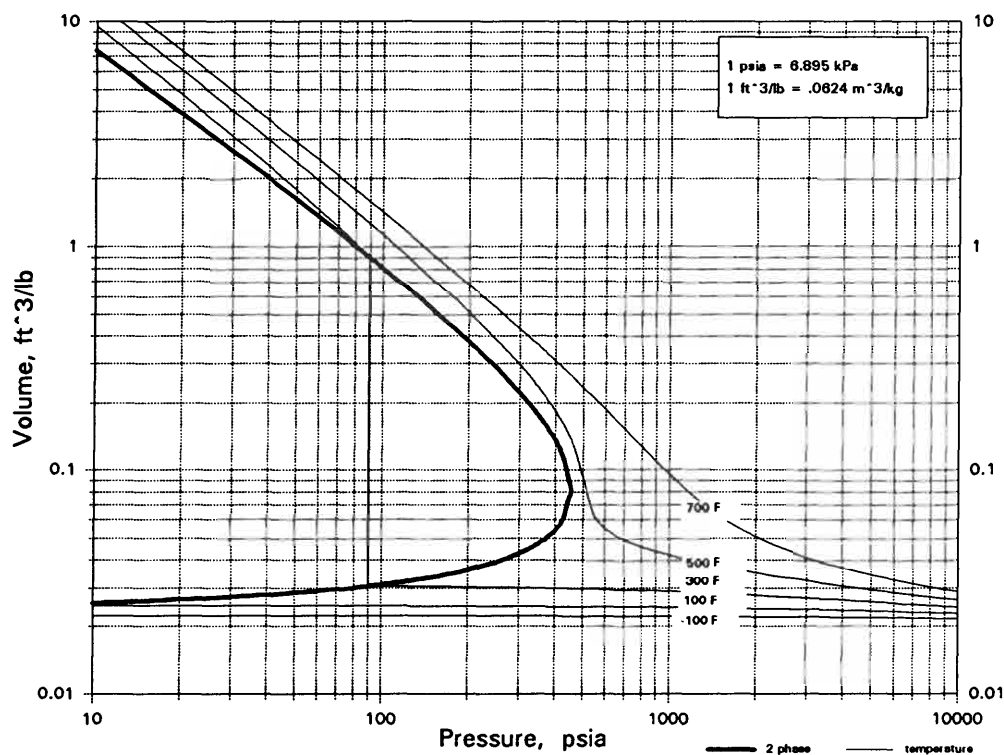
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2-3-DIMETHYL-1-BUTENE



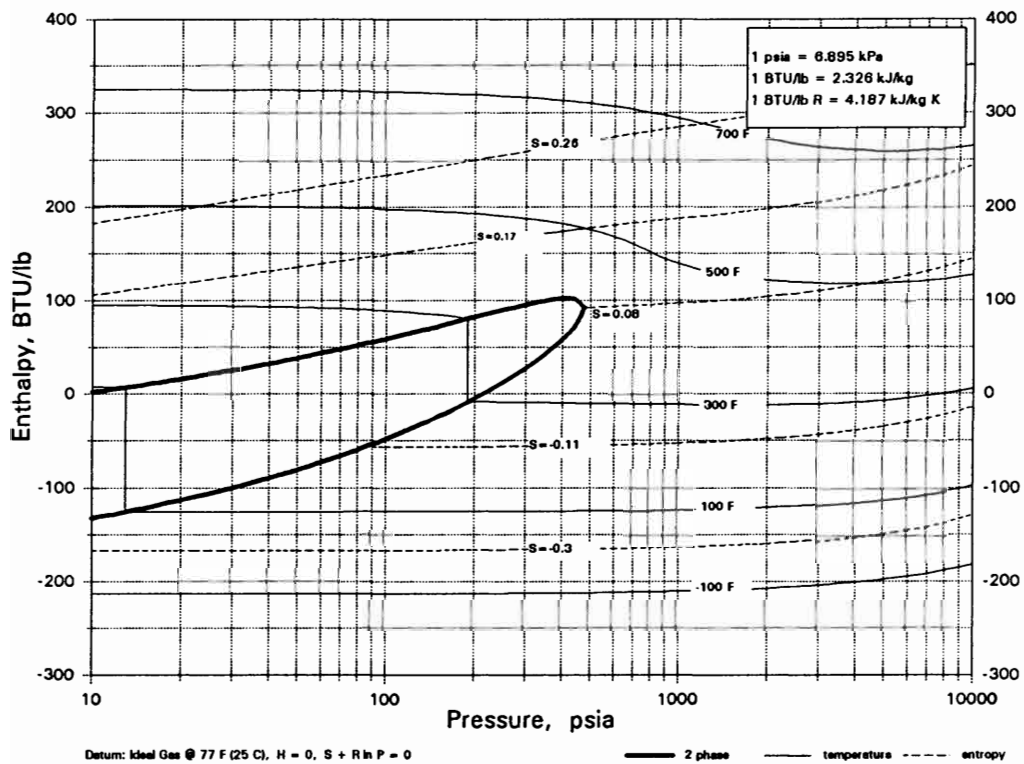
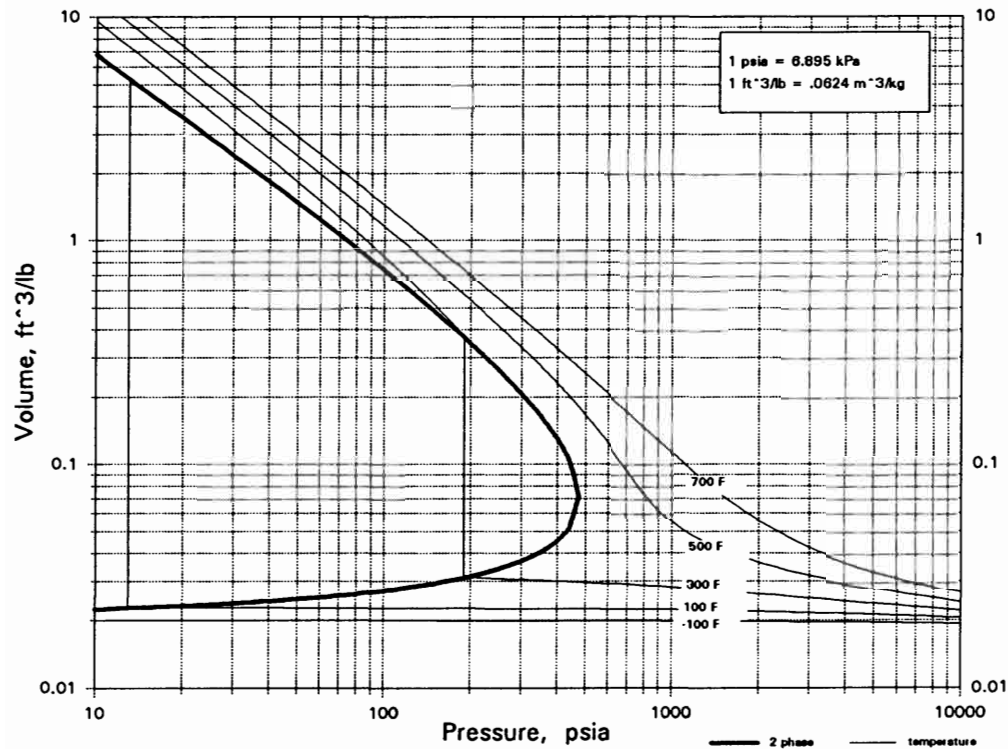
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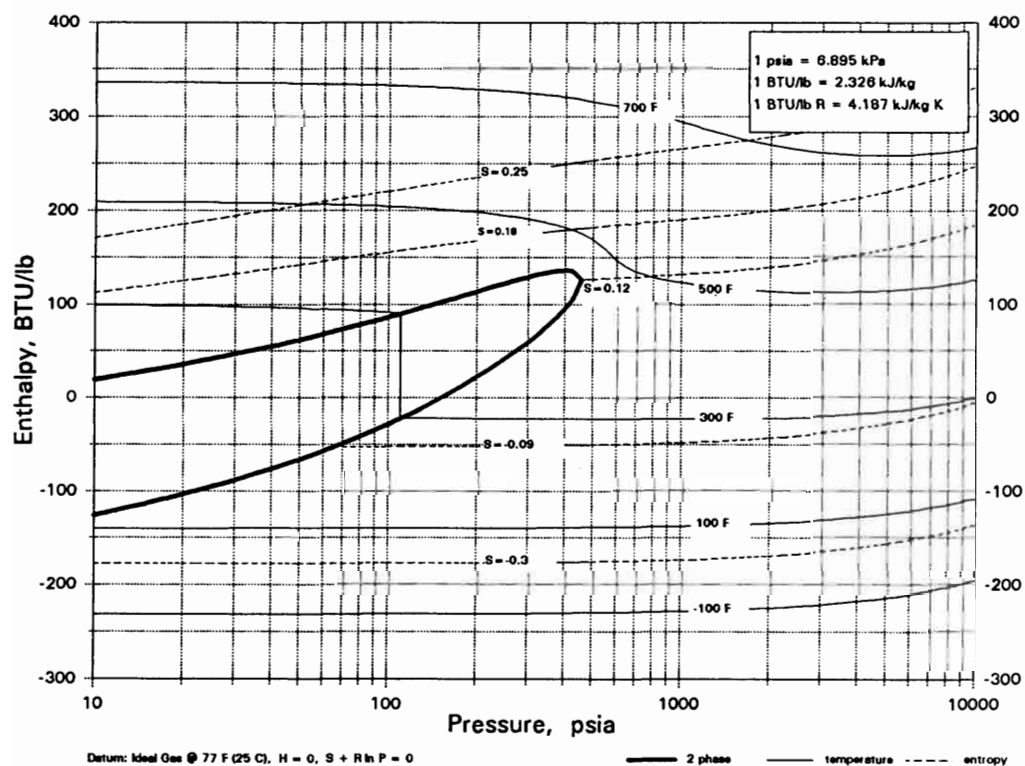
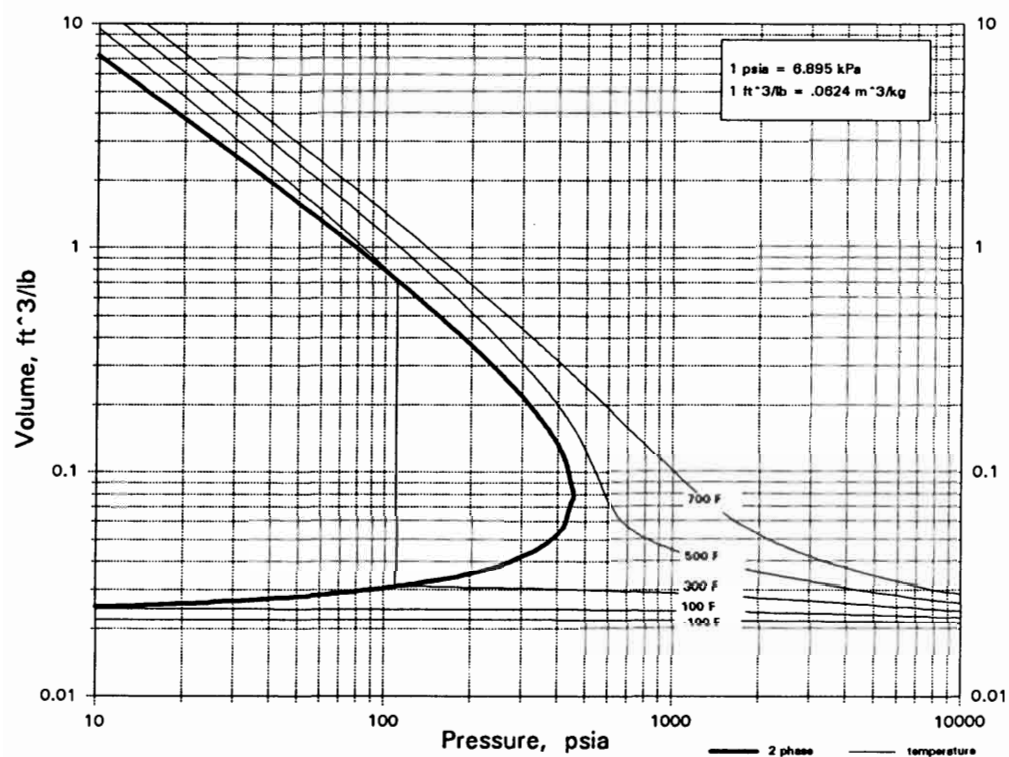
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3-3-DIMETHYL-1-BUTENE



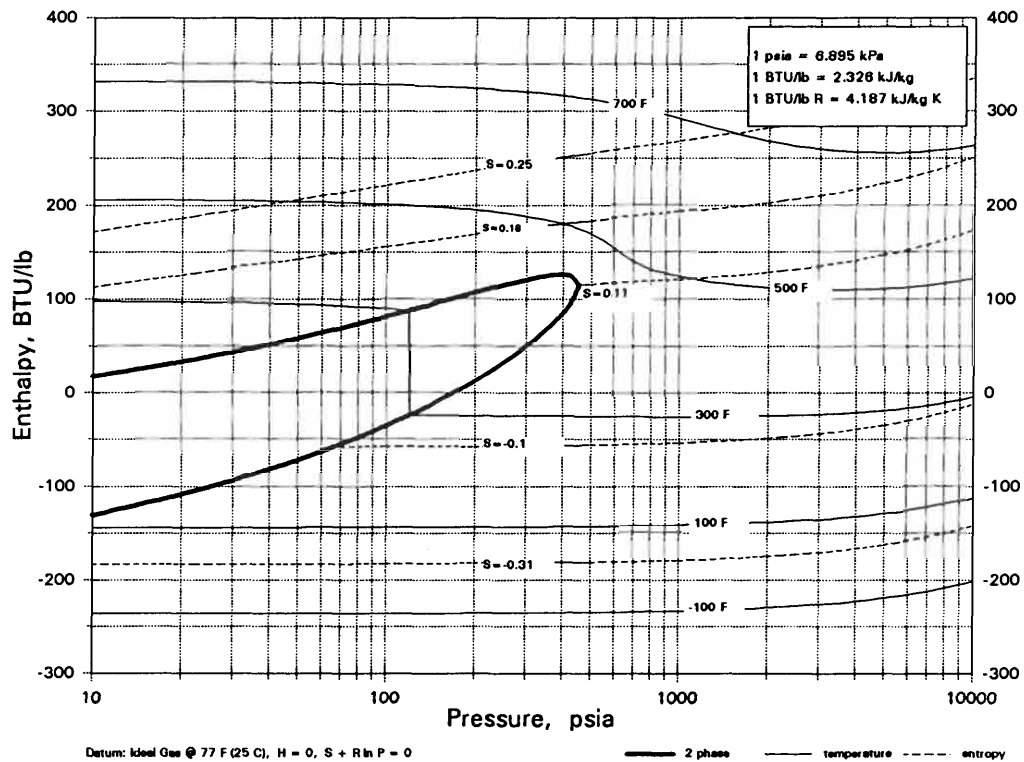
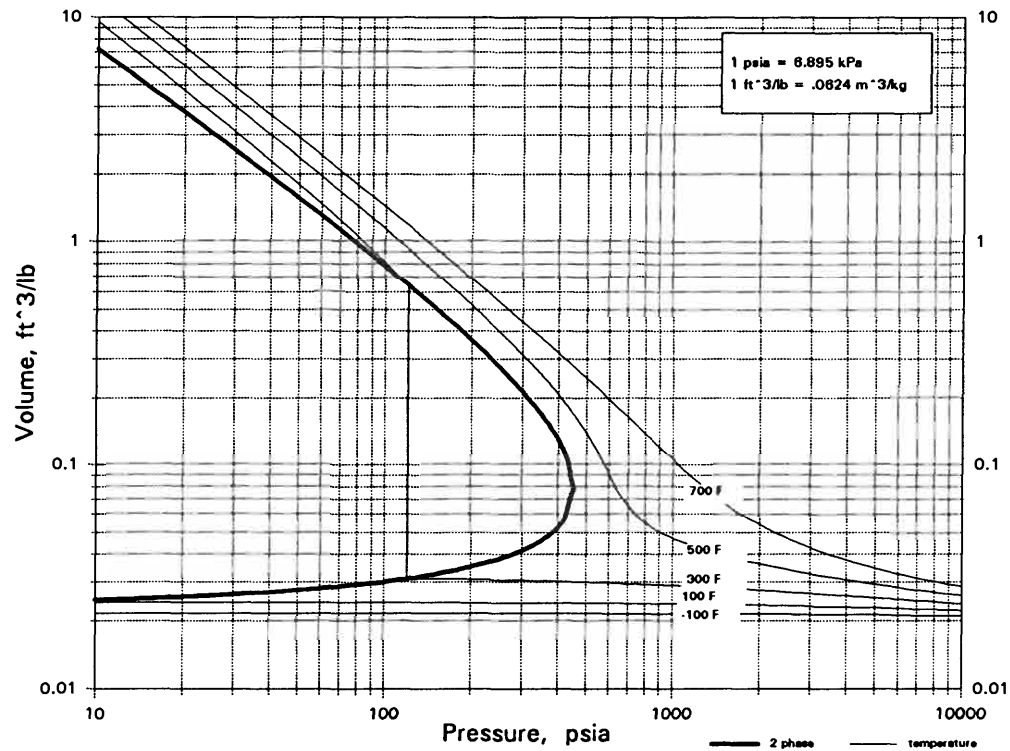
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2-ETHYL-1-BUTENE



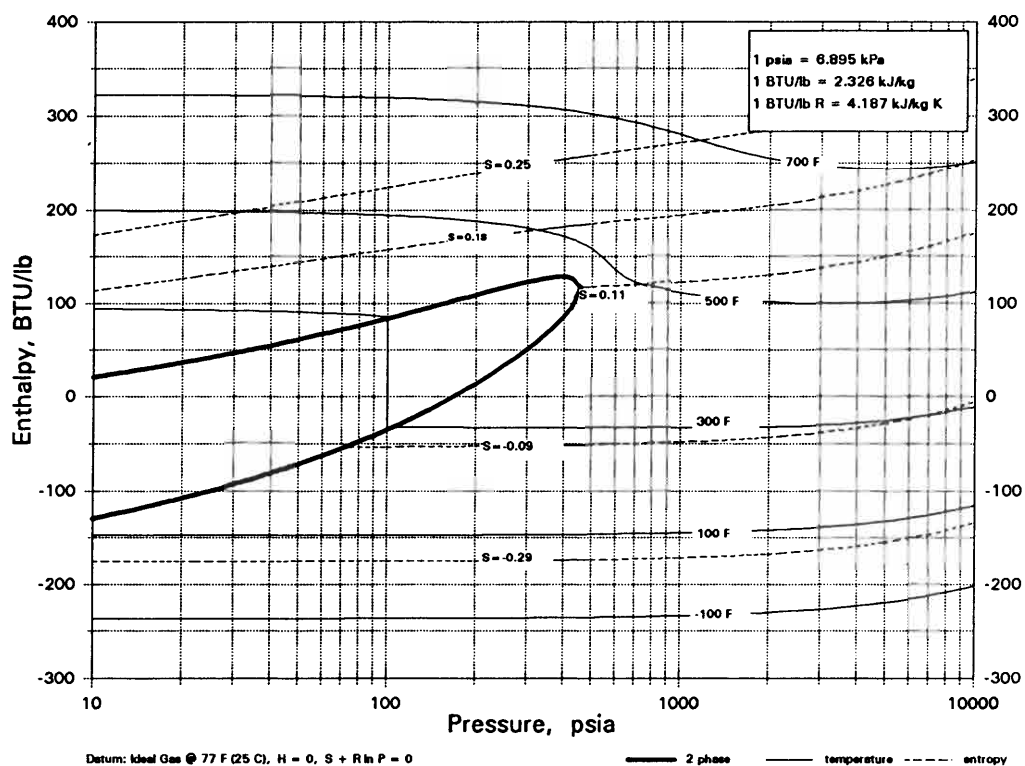
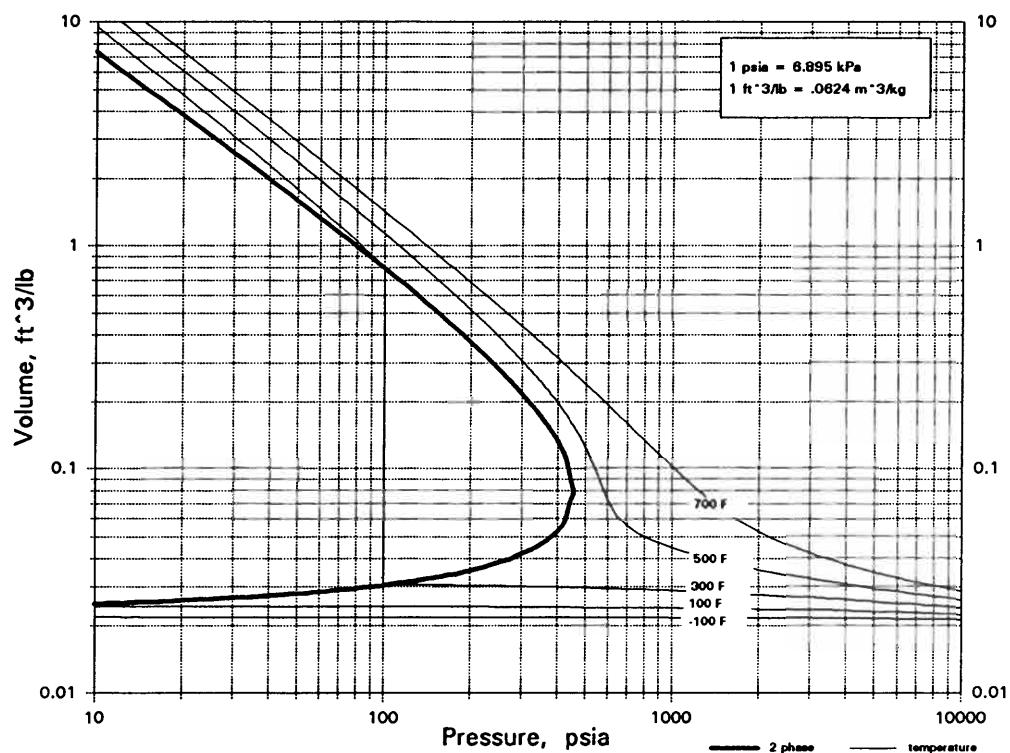
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1-HEXENE



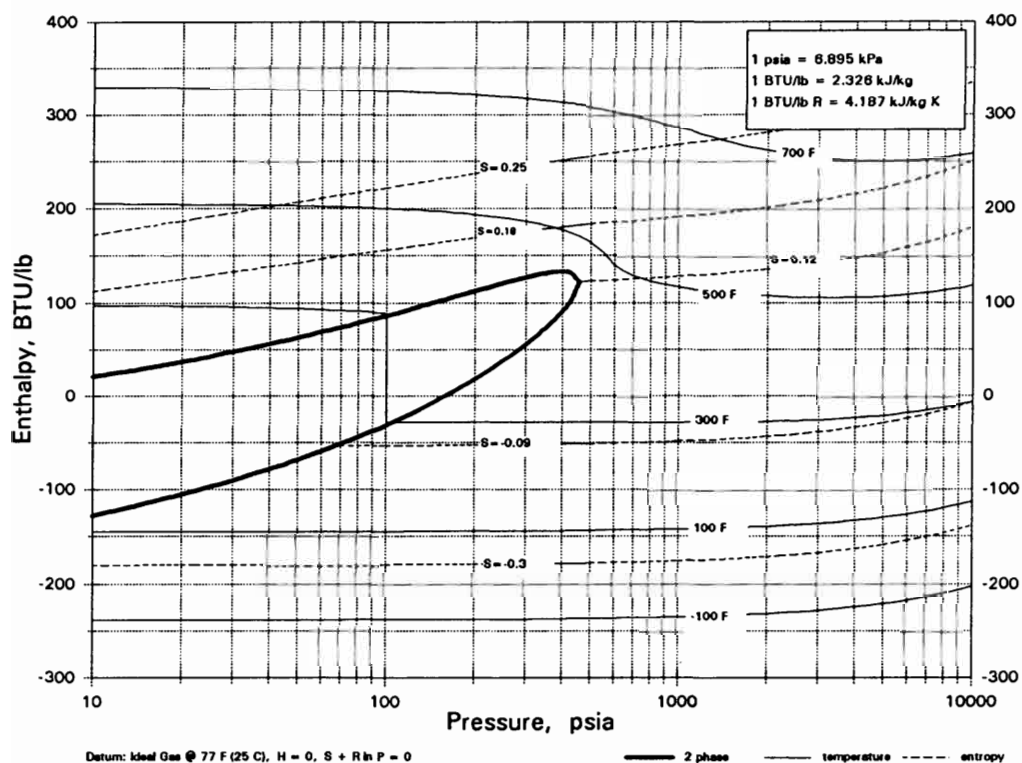
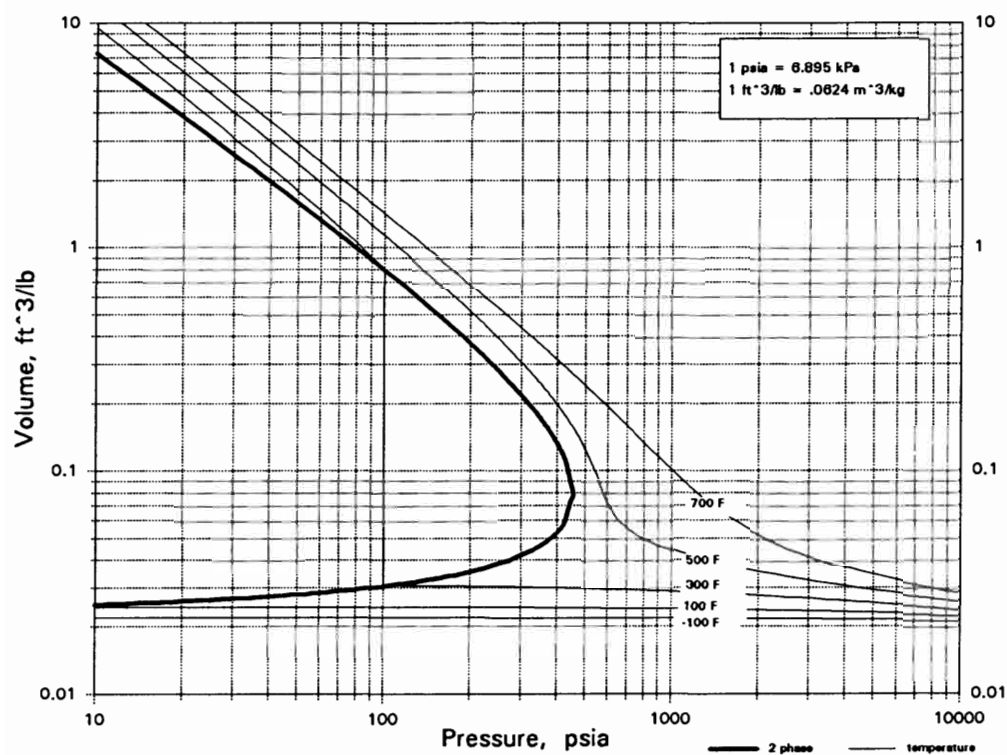
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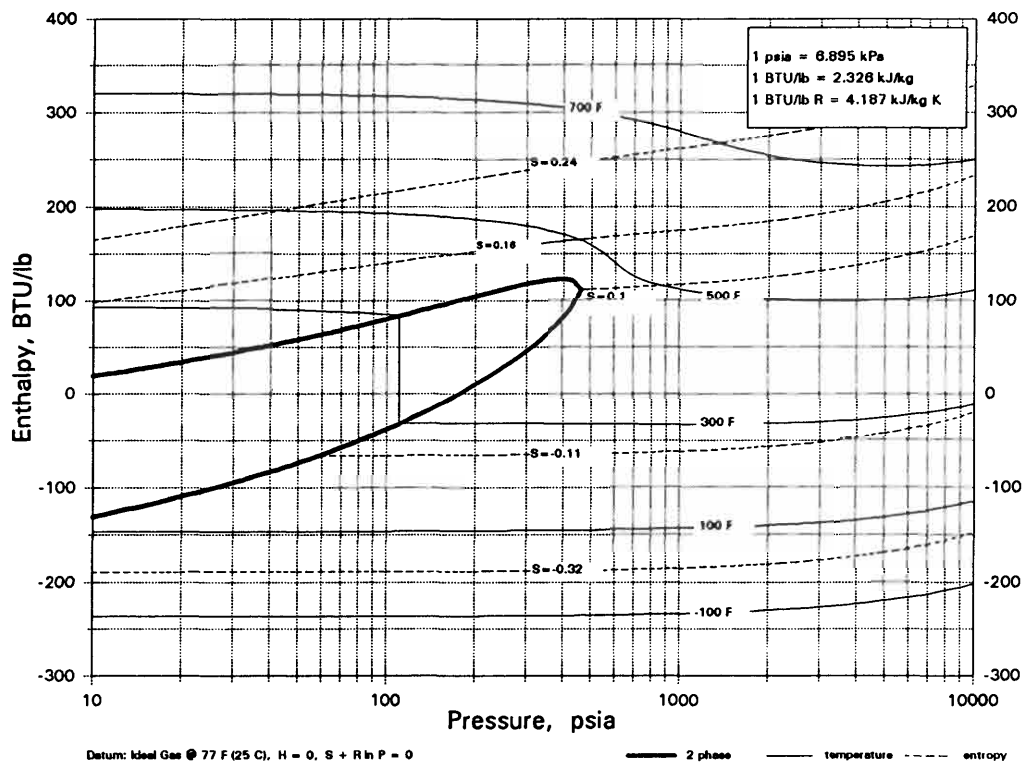
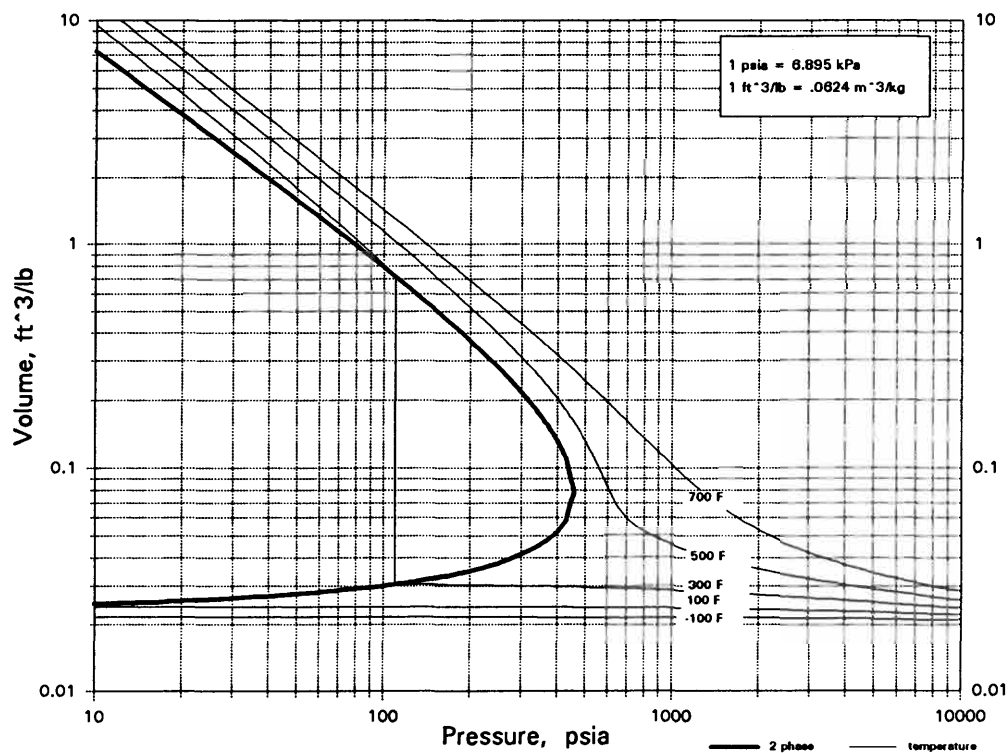


C6H12

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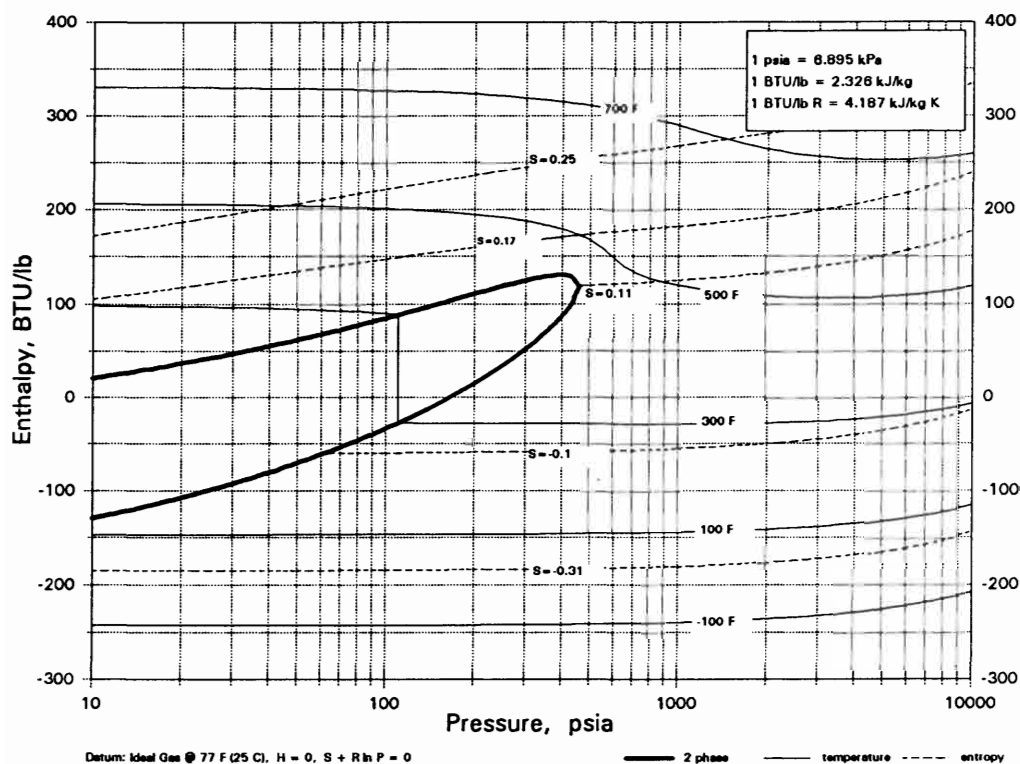
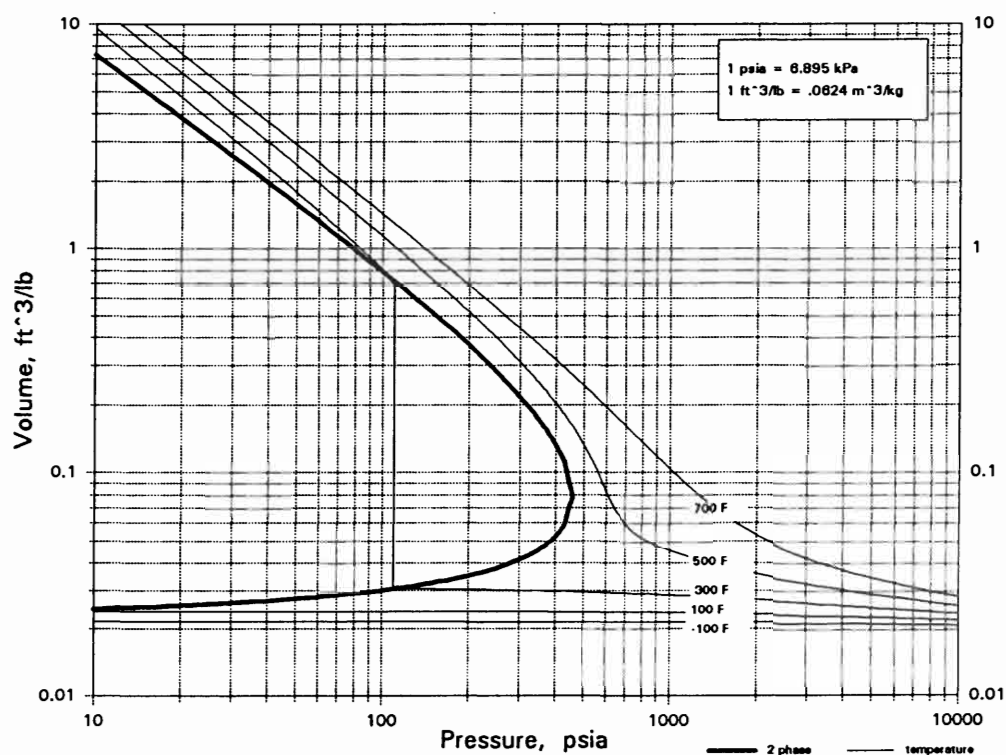


C6H12
cis-3-HEXENE



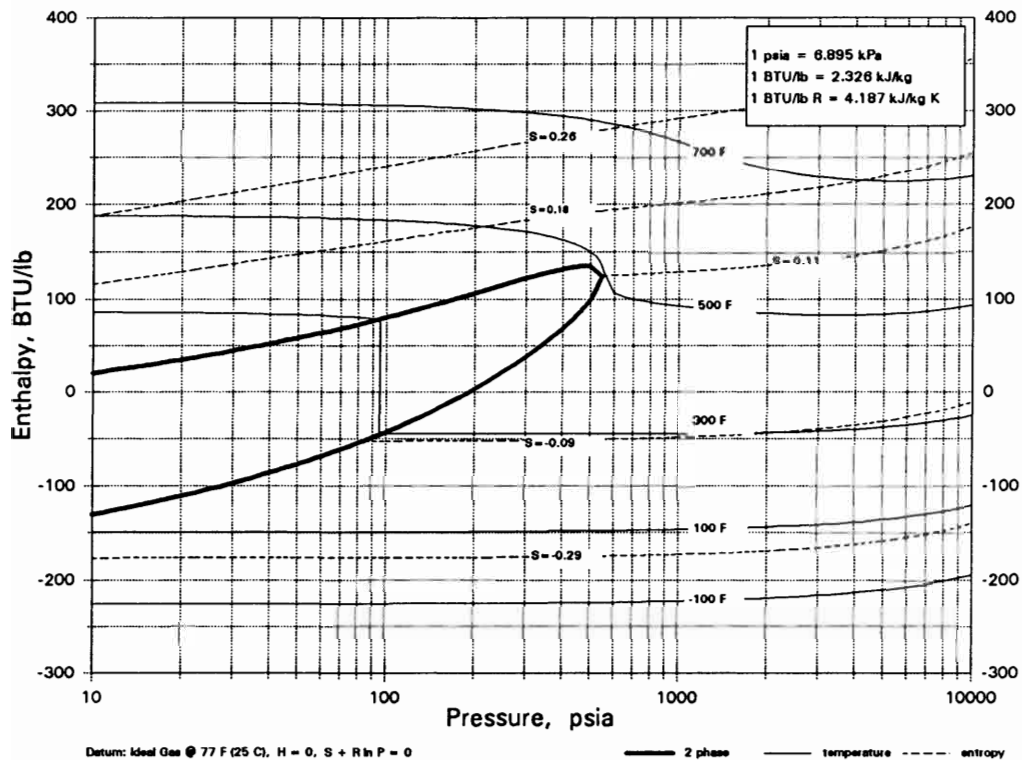
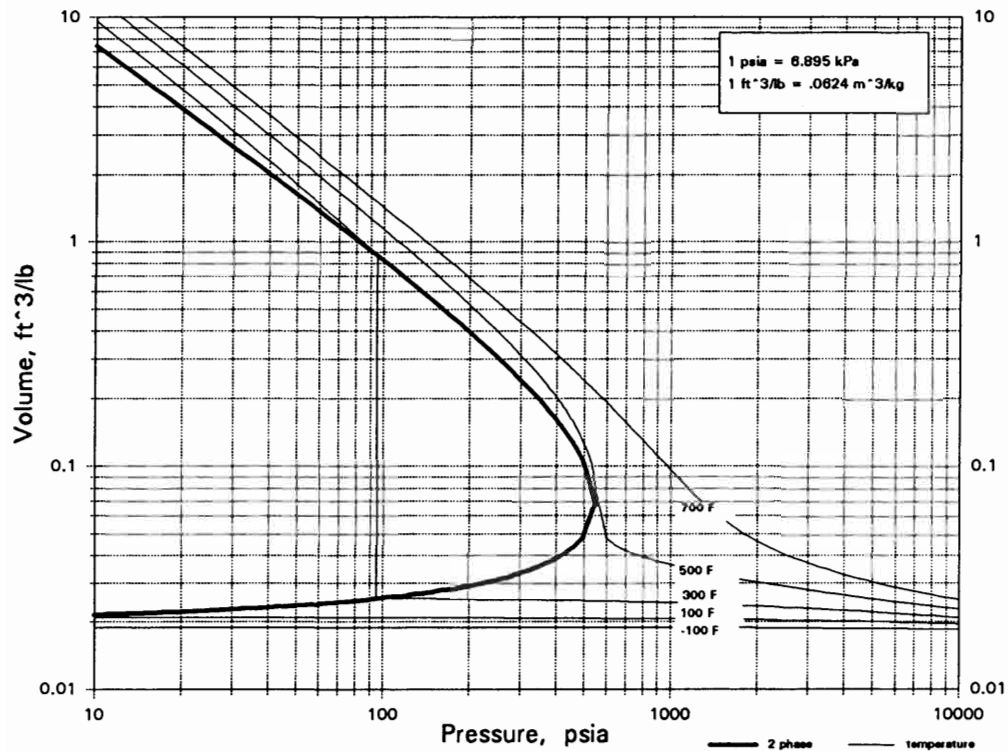
C6H12

trans-3-HEXENE



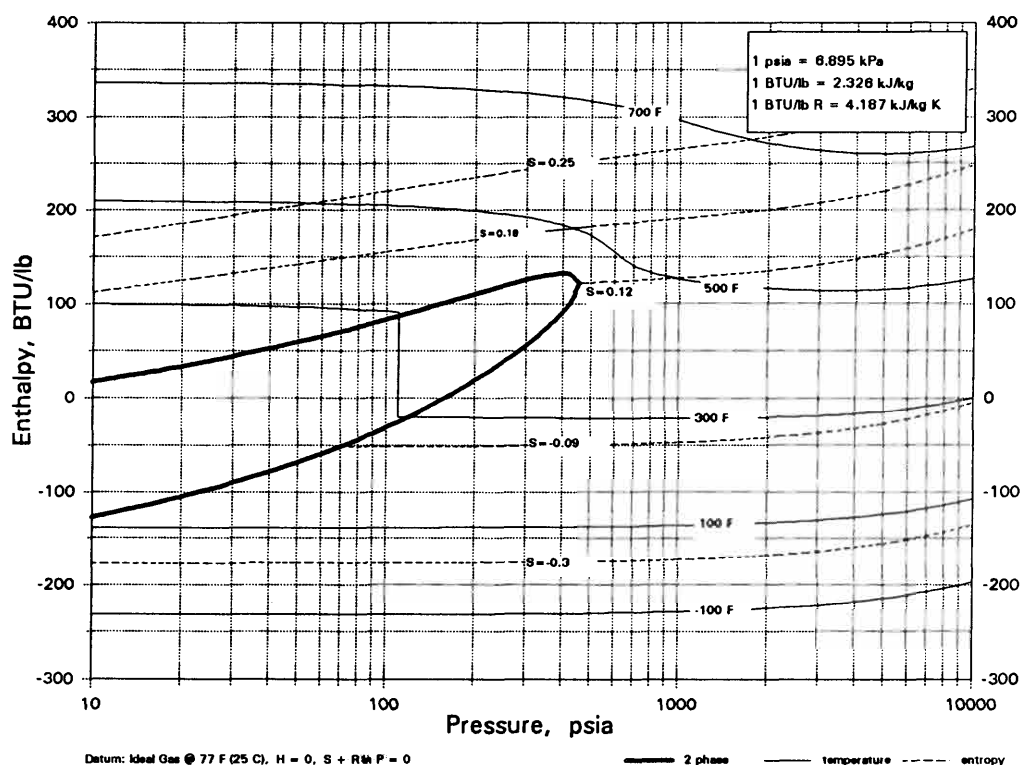
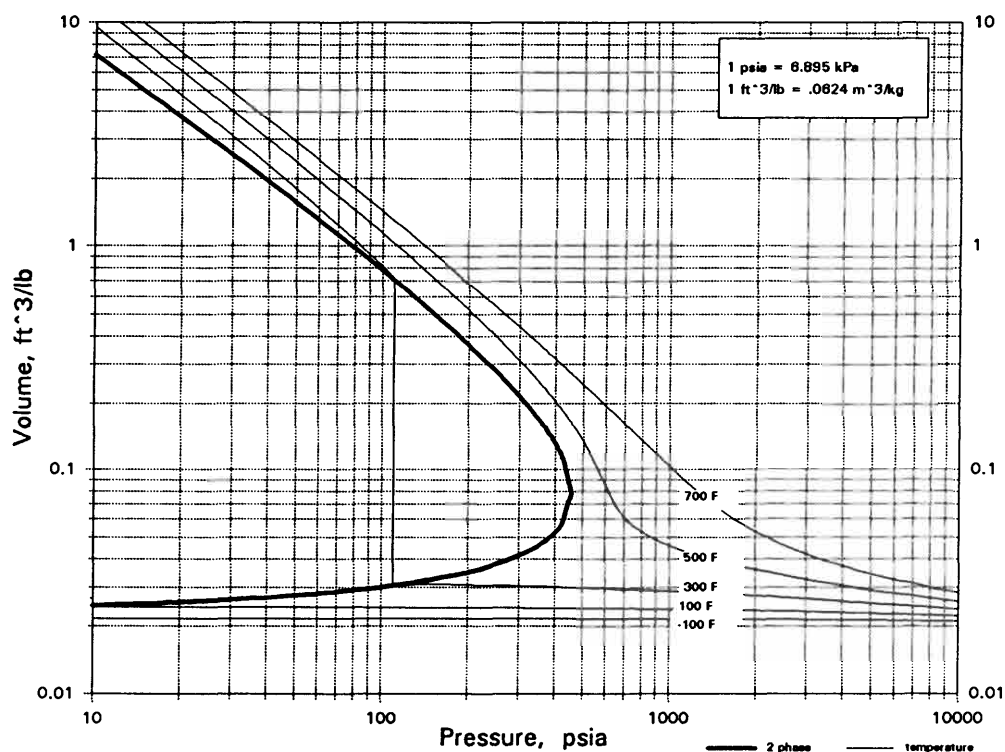
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METHYLCYCLOPENTANE



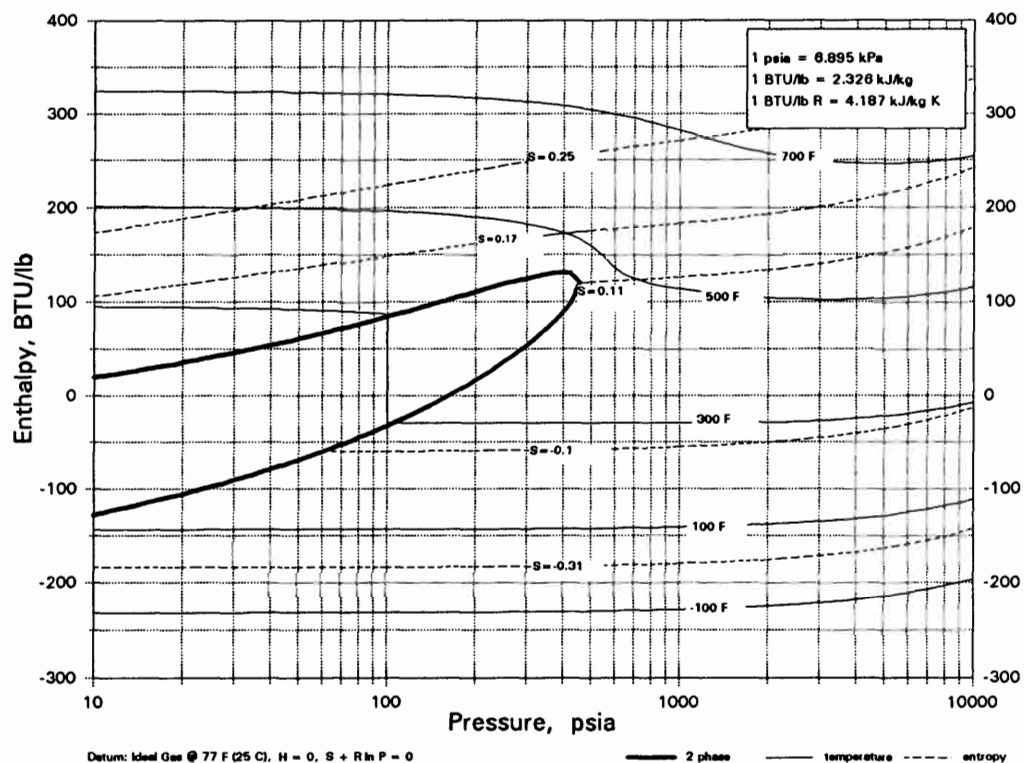
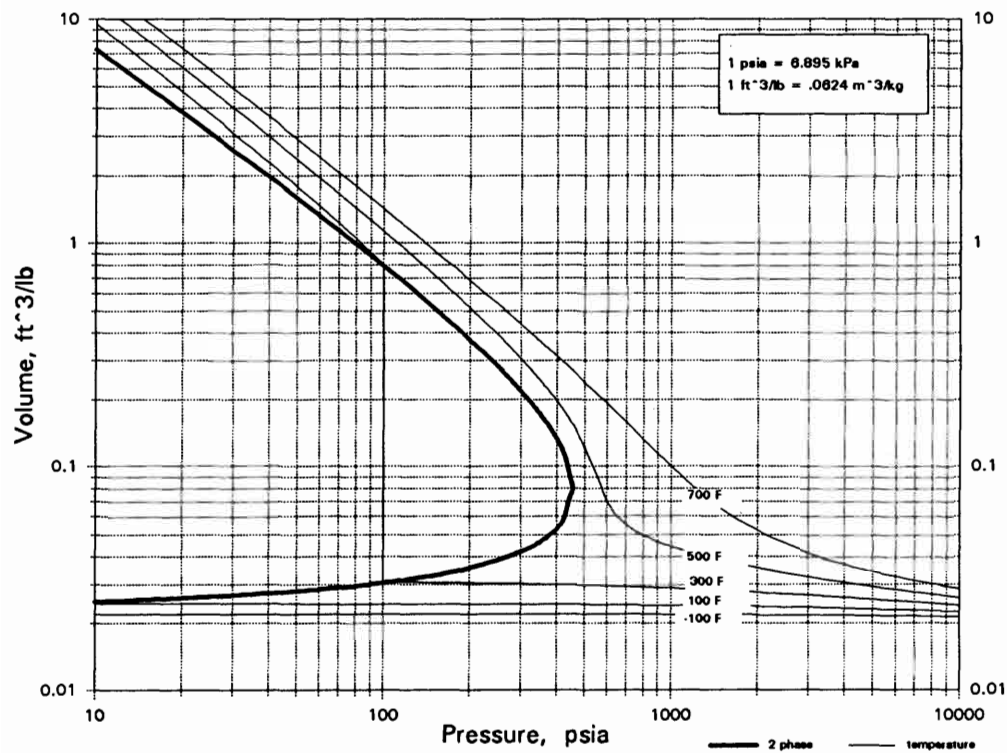
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2-METHYL-1-PENTENE



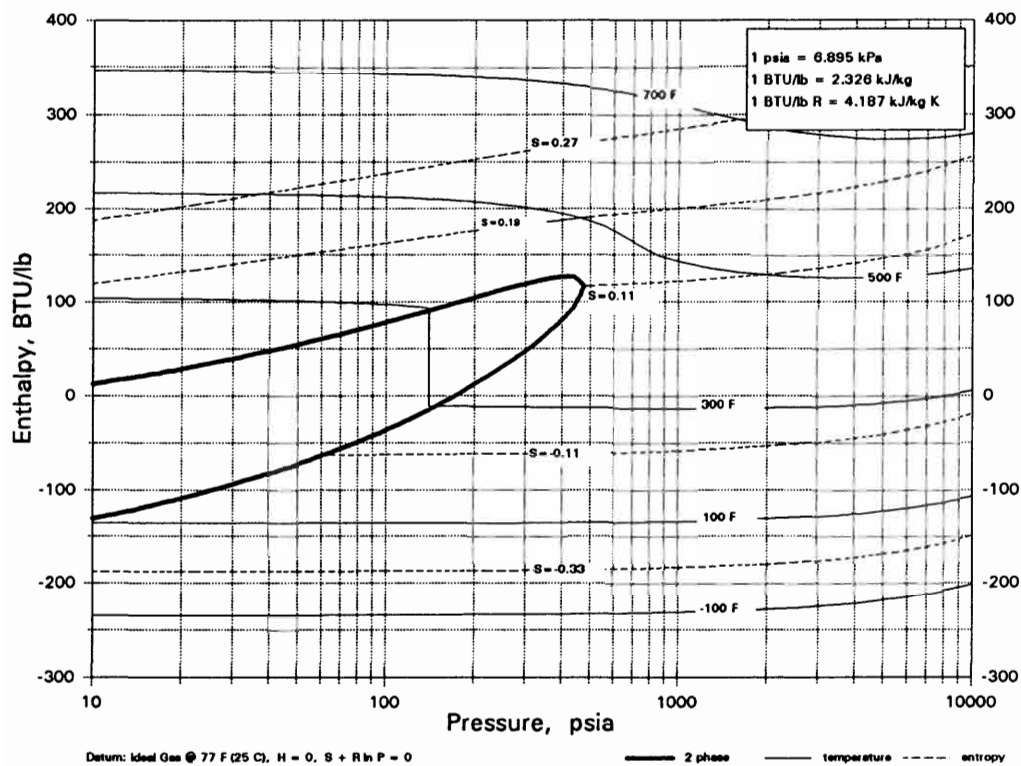
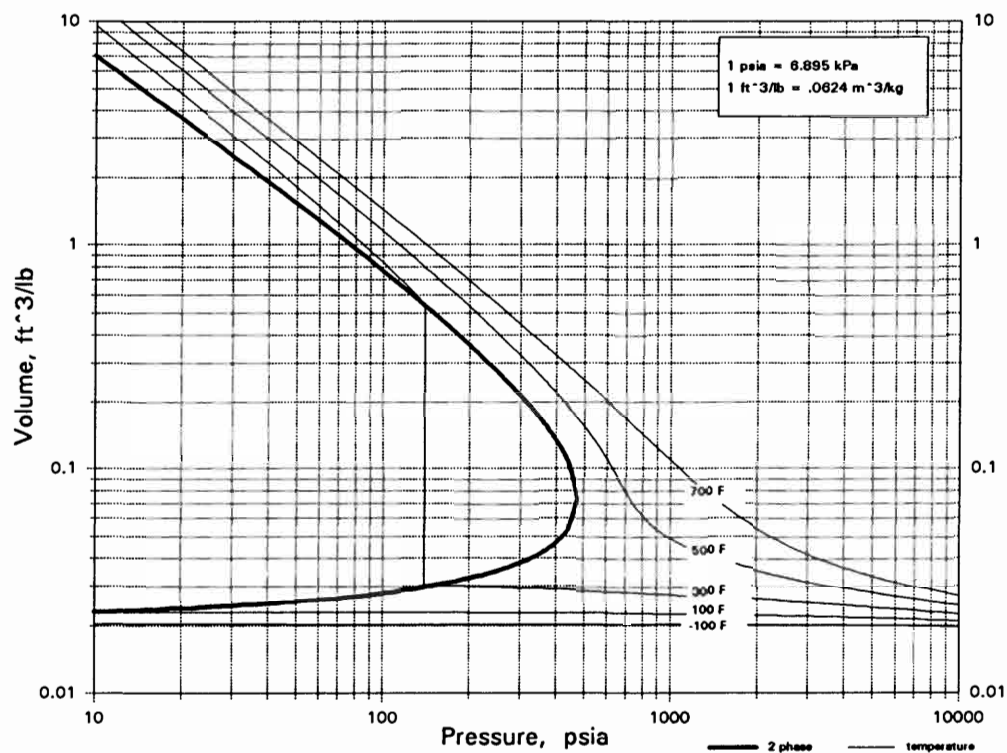
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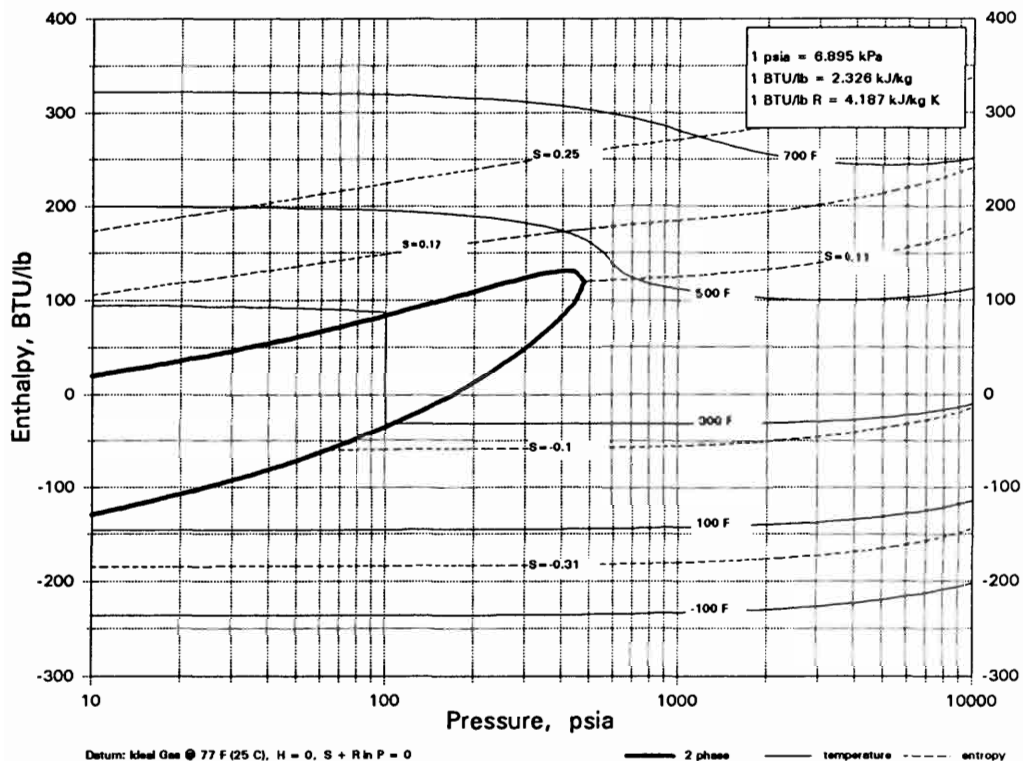
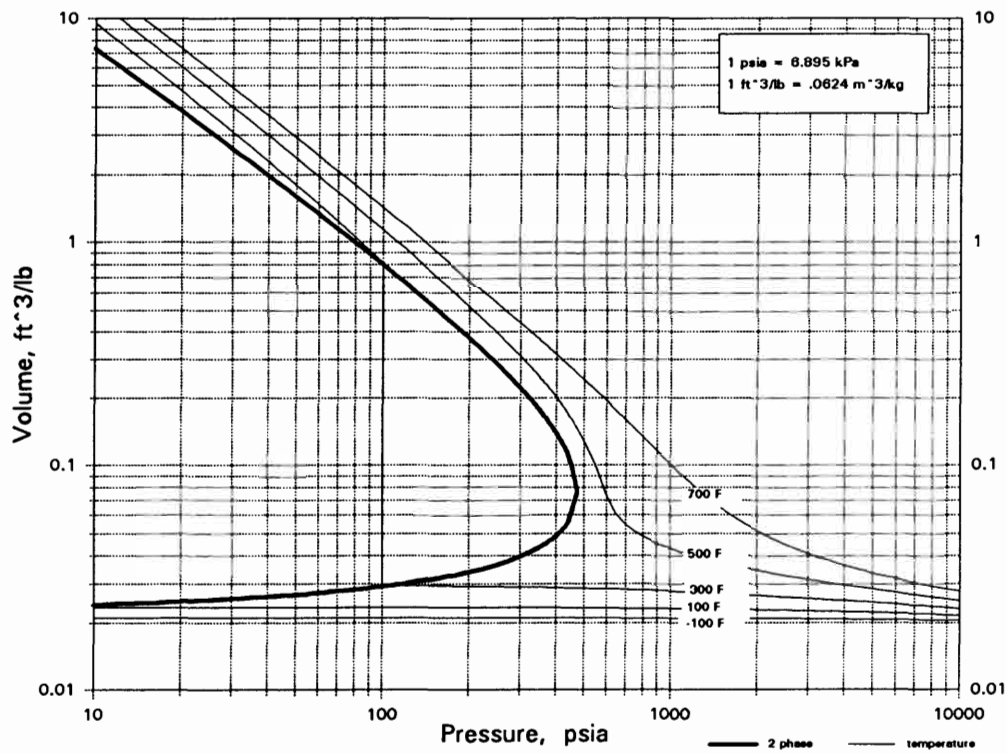
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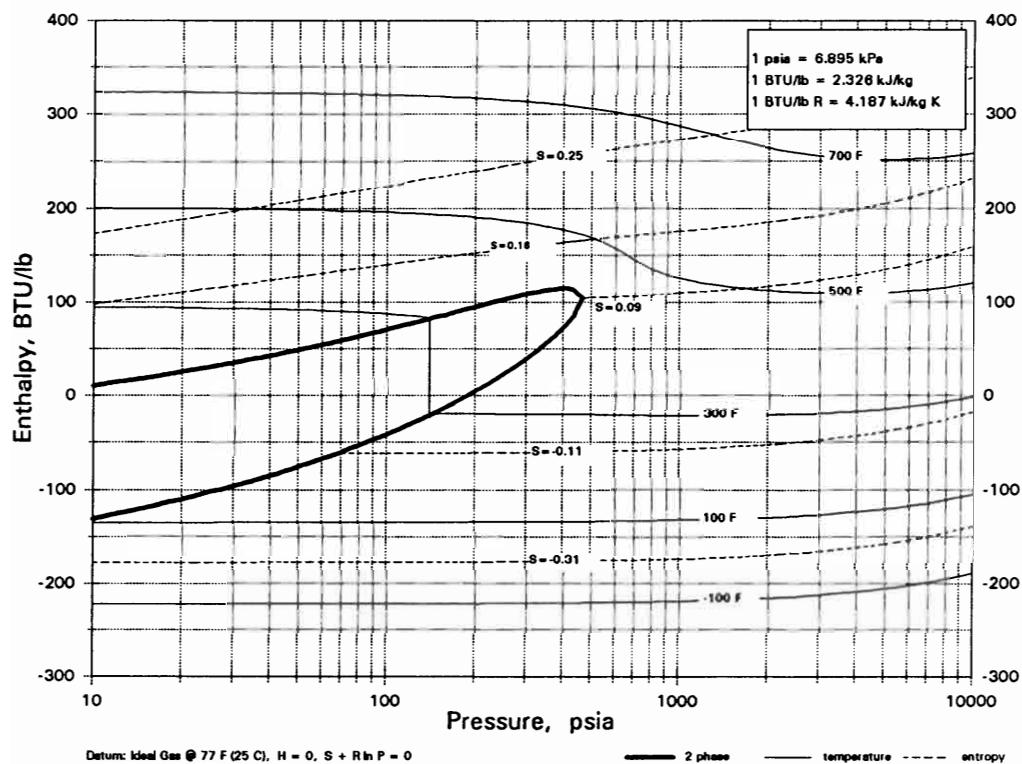
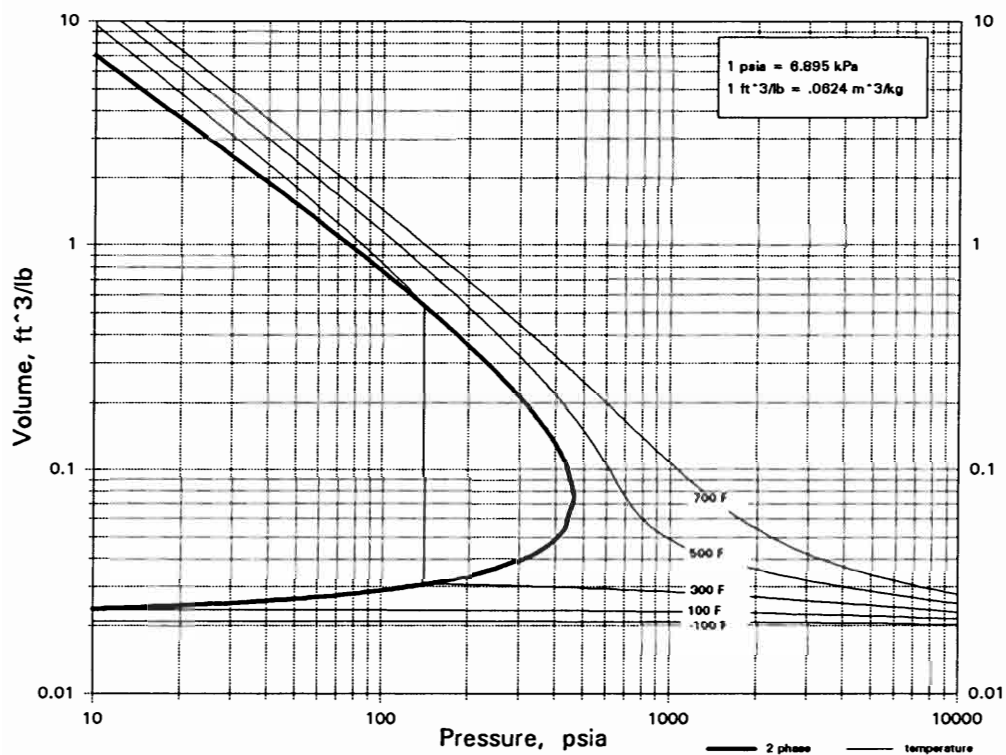
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3-METHYL-cis-2-PENTENE



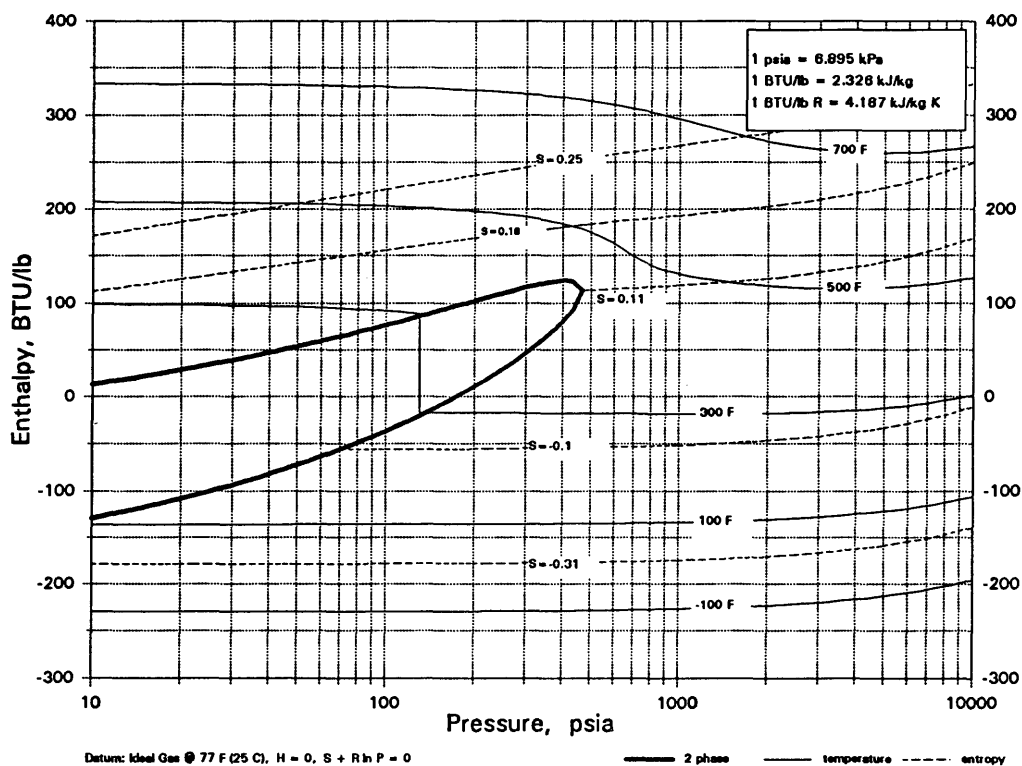
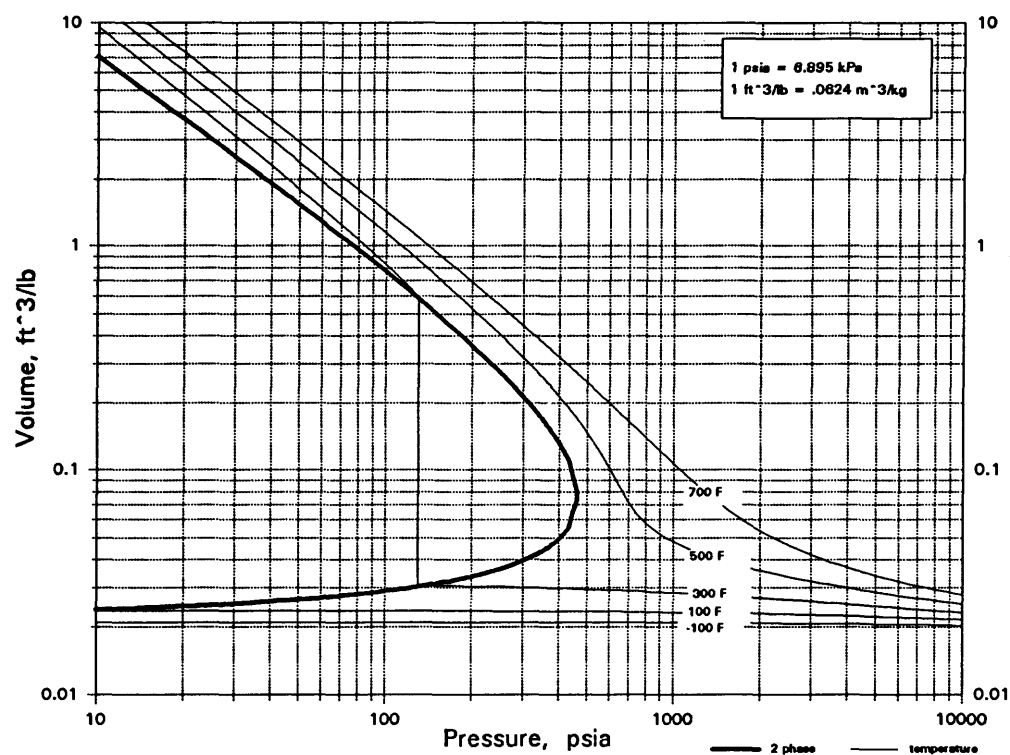
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4-METHYL-1-PENTENE



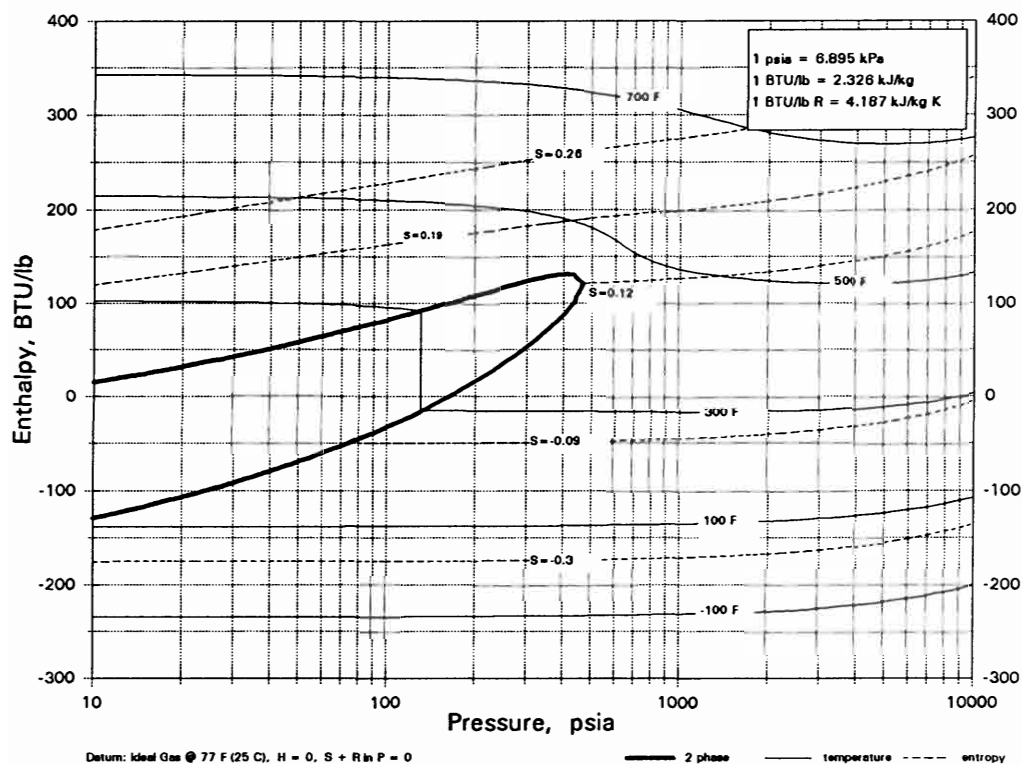
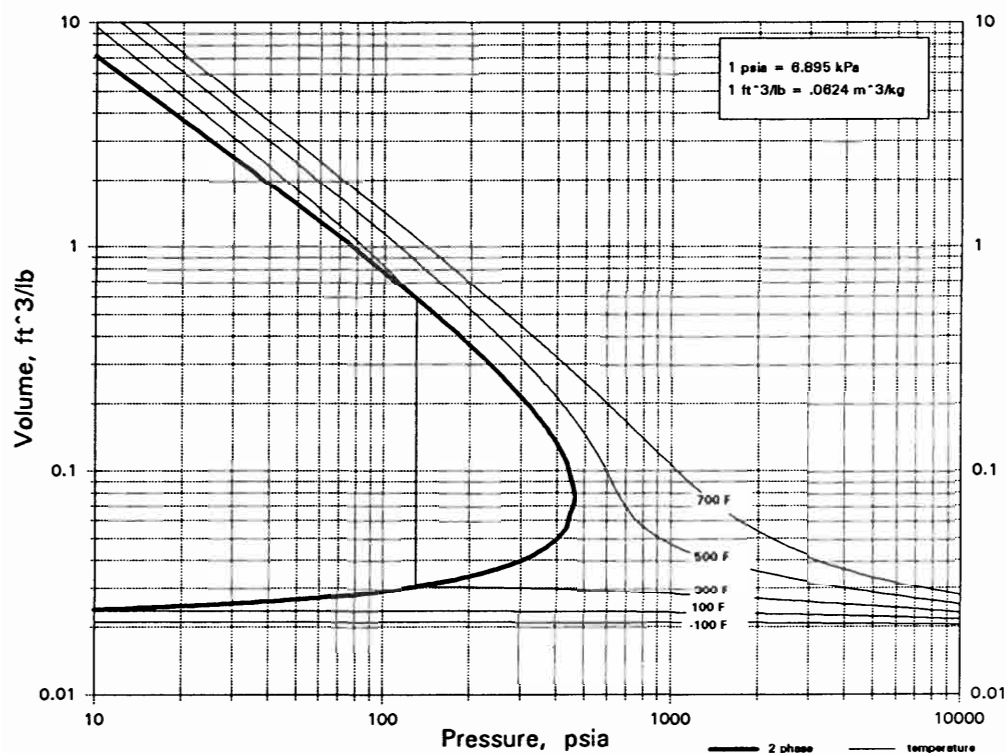
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4-METHYL-cis-2-PENTENE



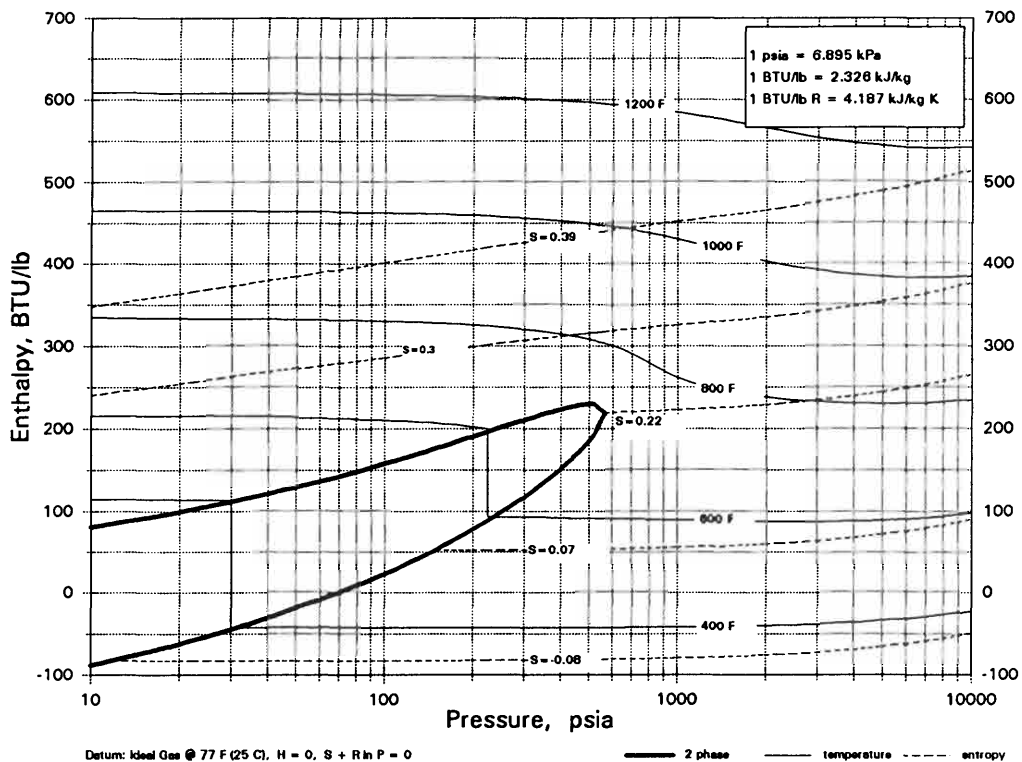
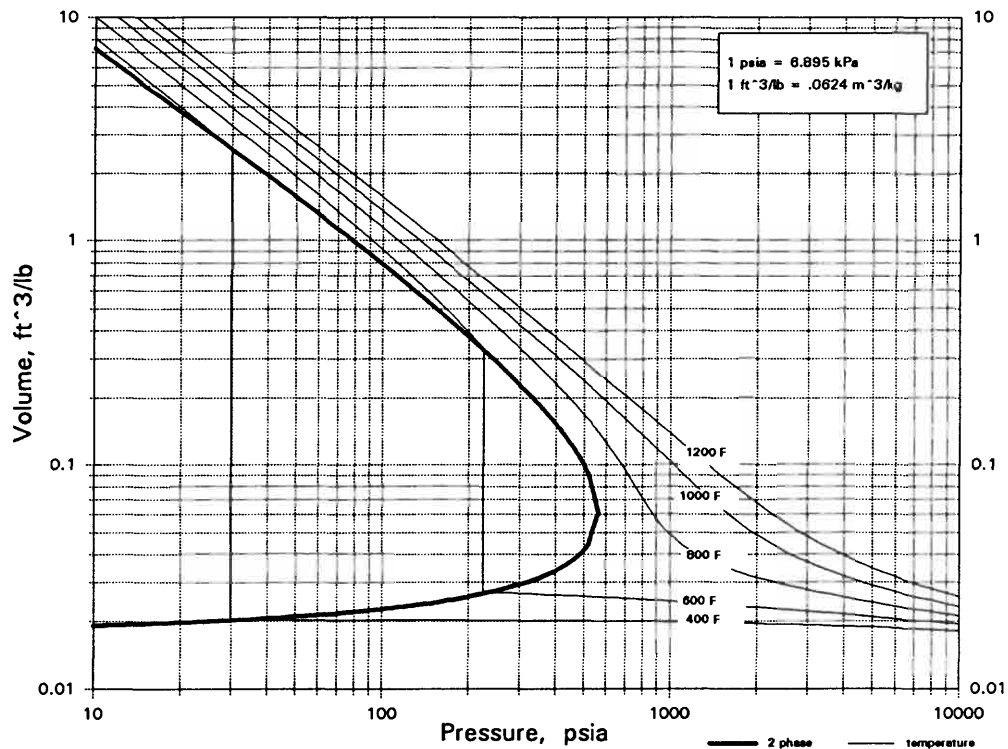
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4-METHYL-trans-2-PENTENE



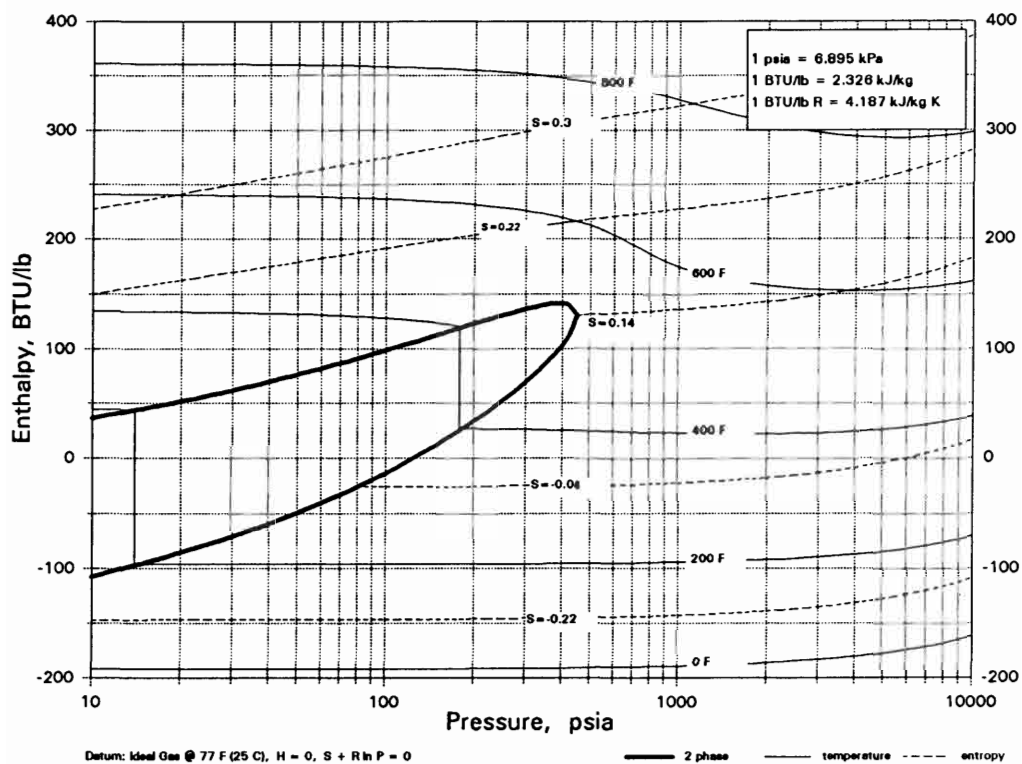
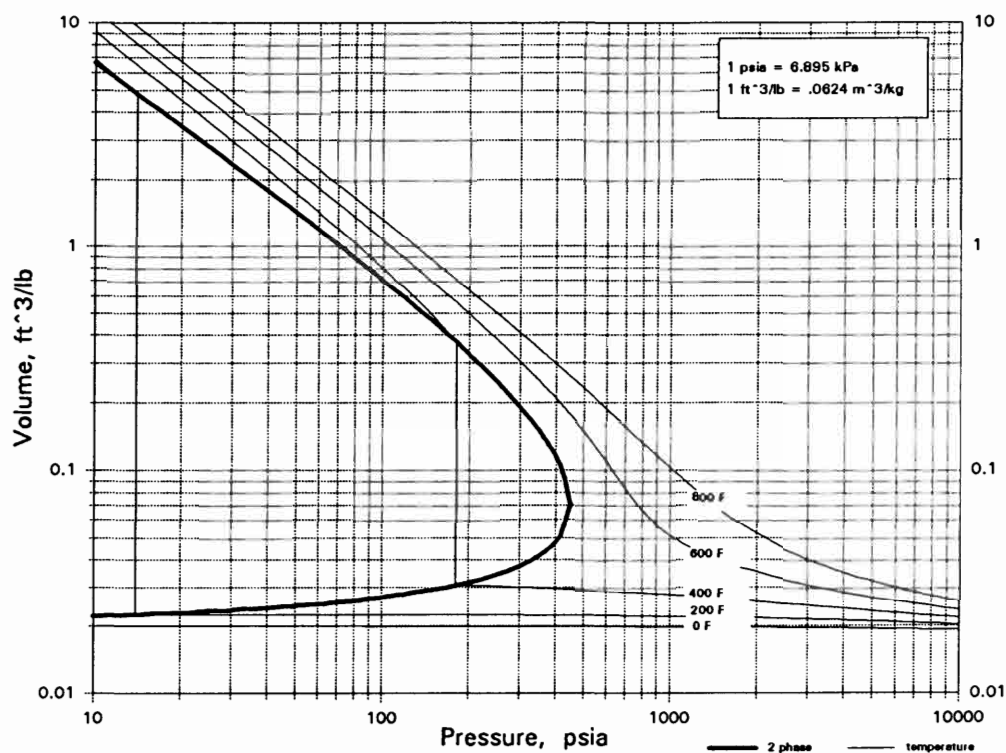
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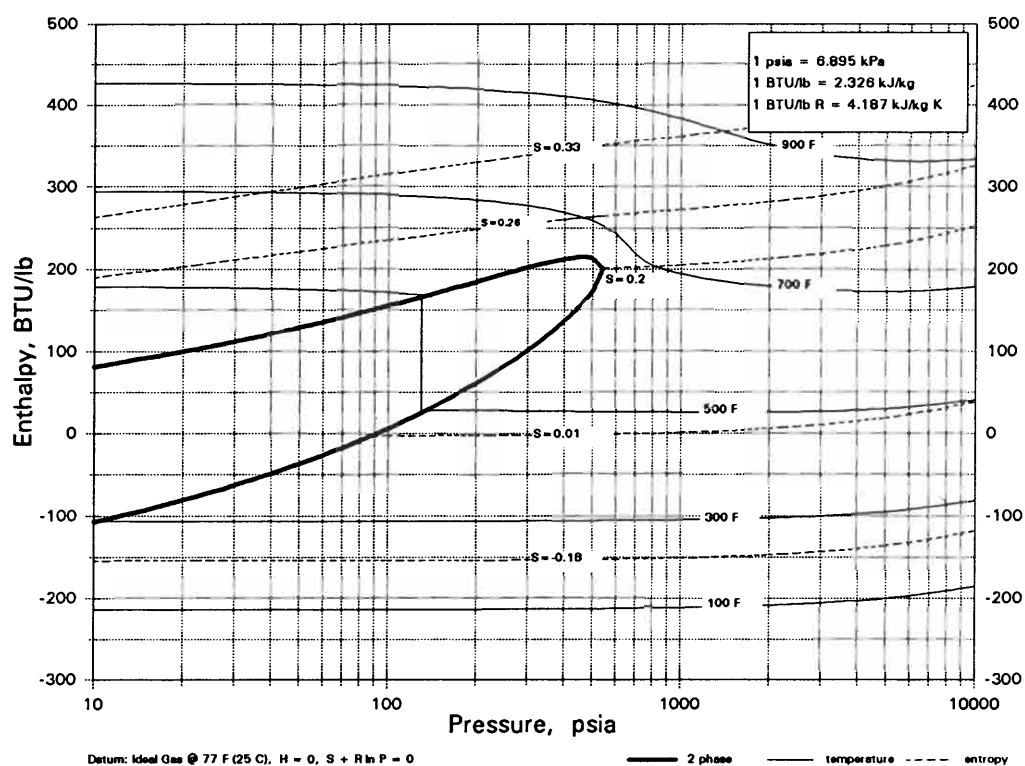
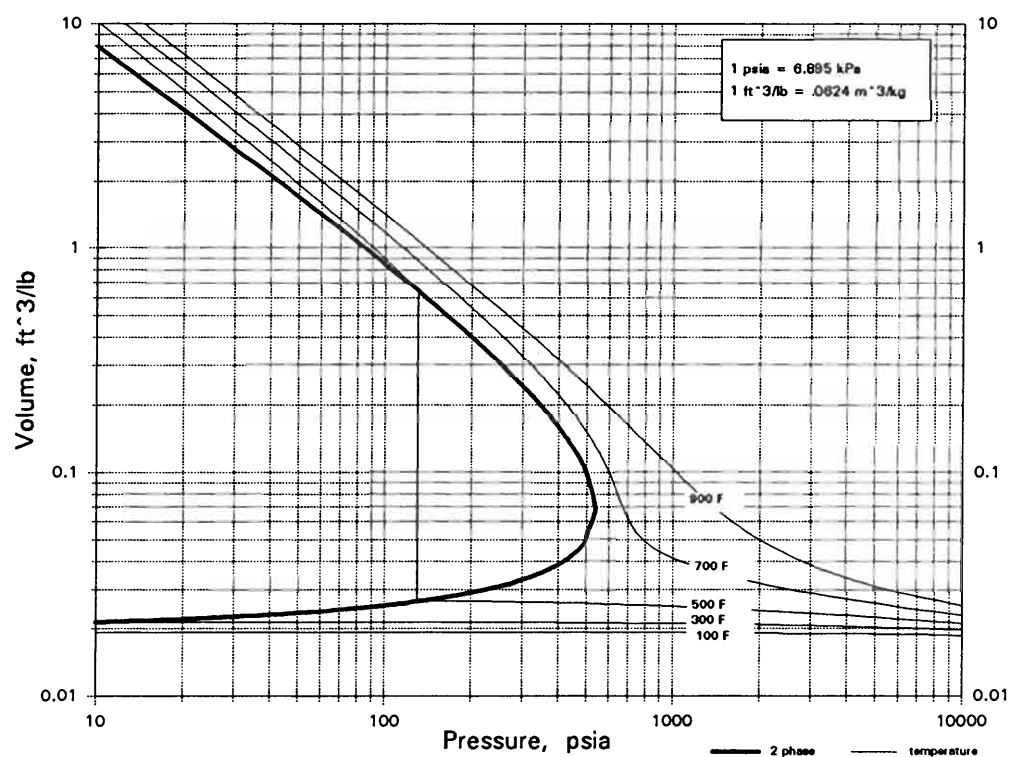
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BUTYL VINYL ETHER



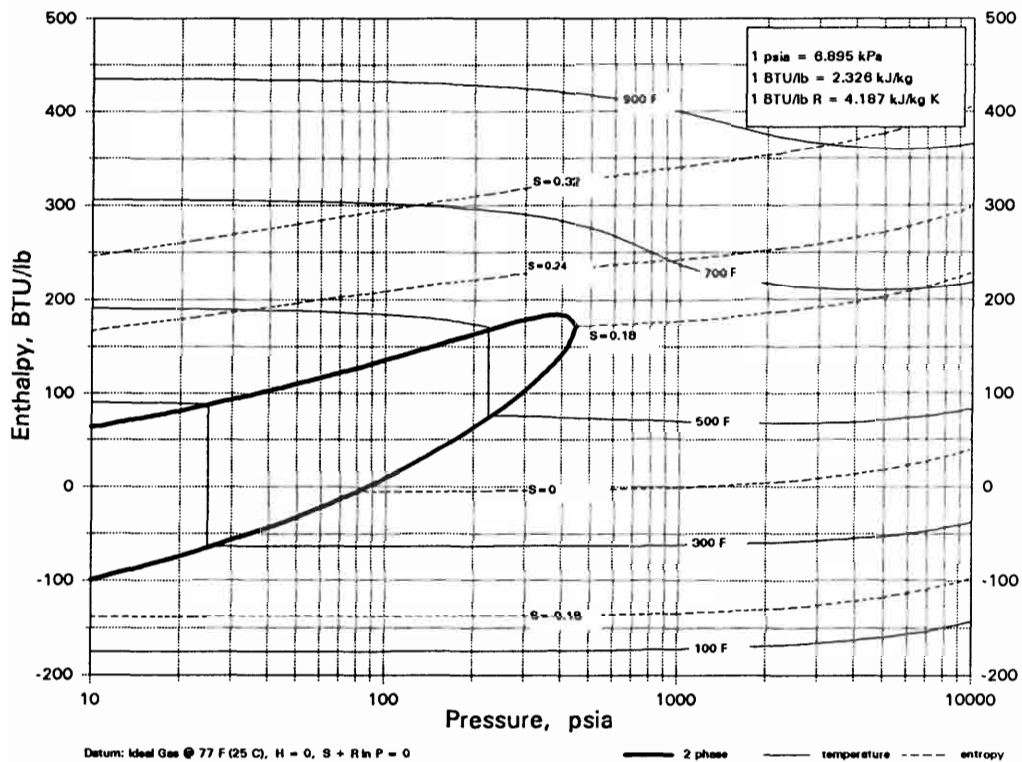
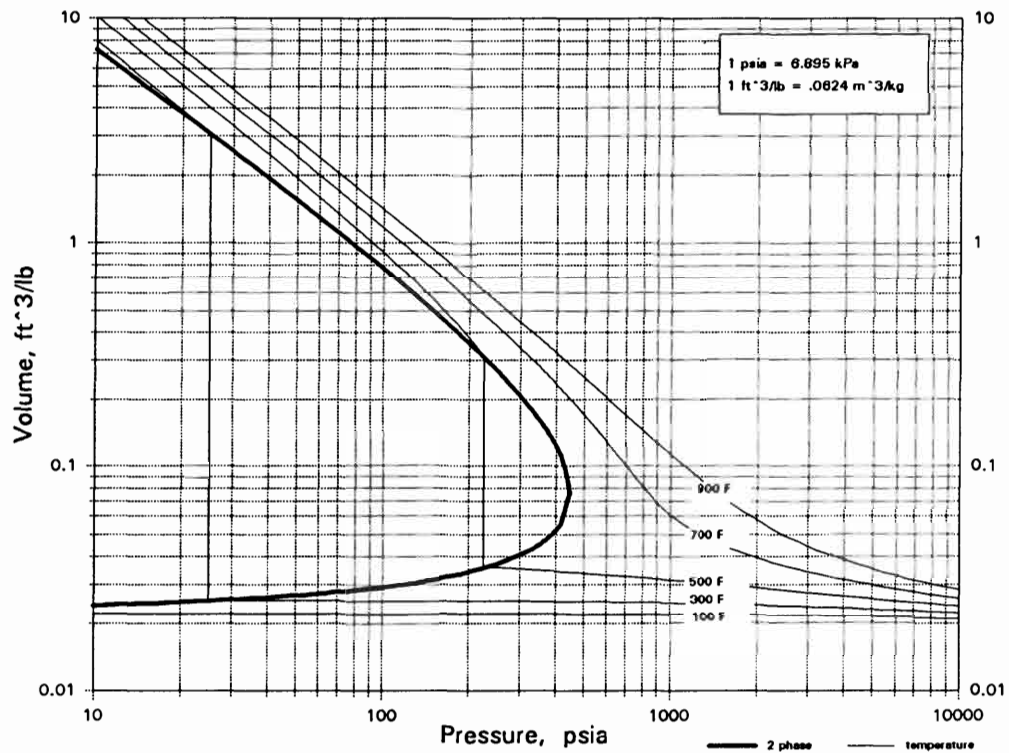
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CYCLOHEXANOL



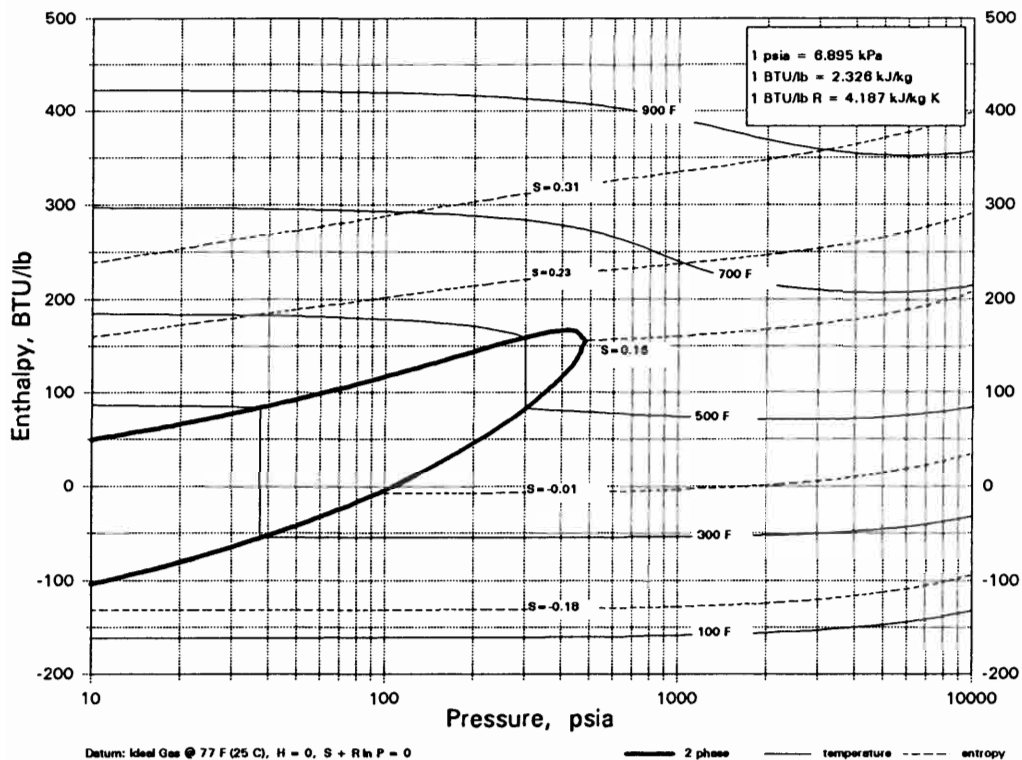
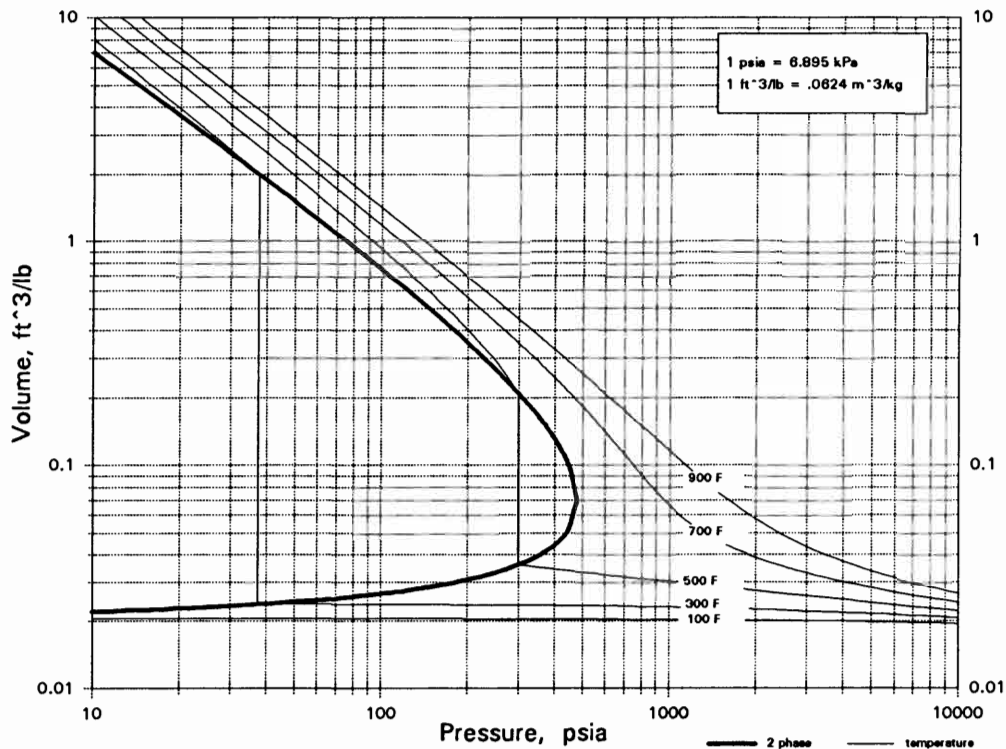
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1-HEXANAL



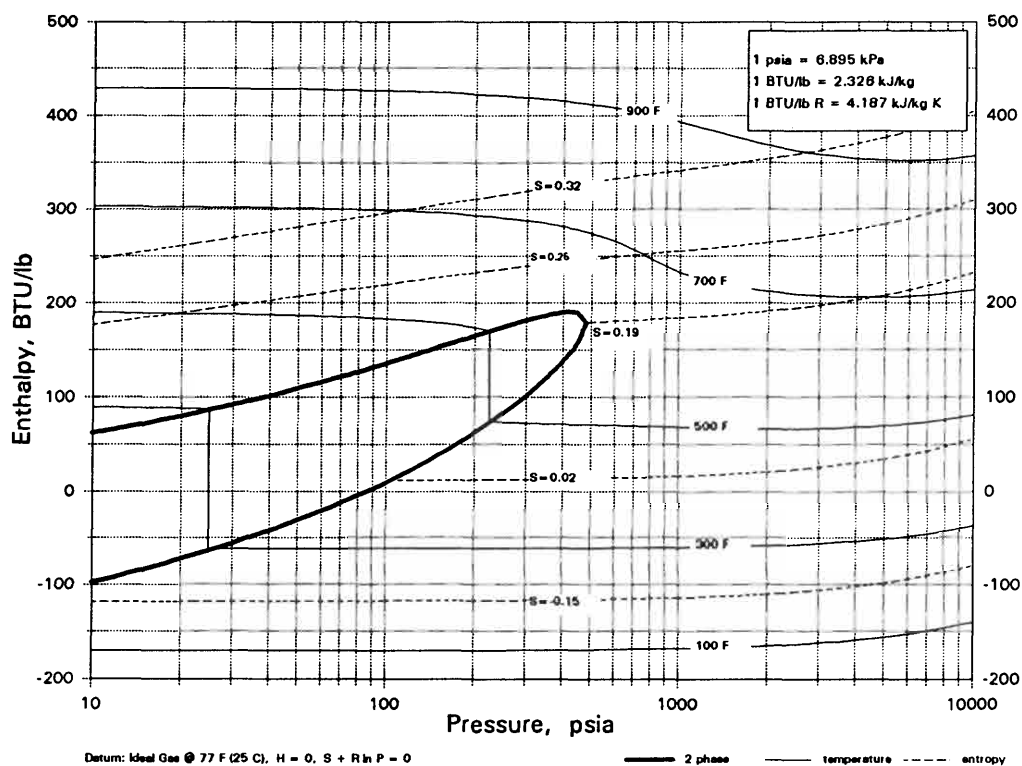
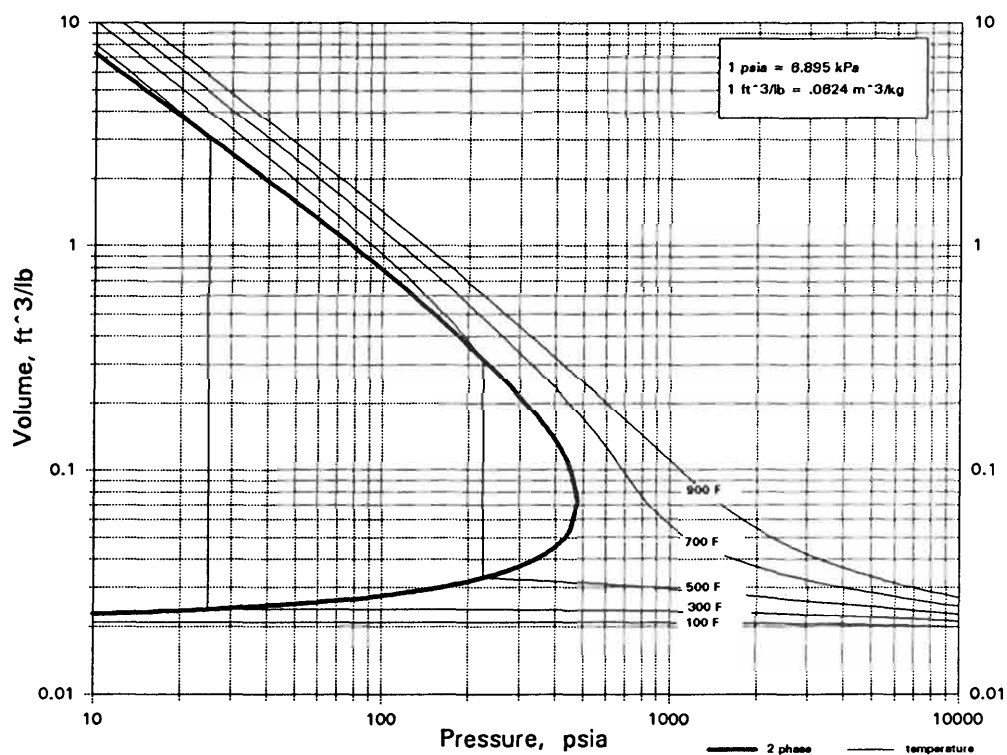
C6H12O

ETHYL ISOPROPYL KETONE



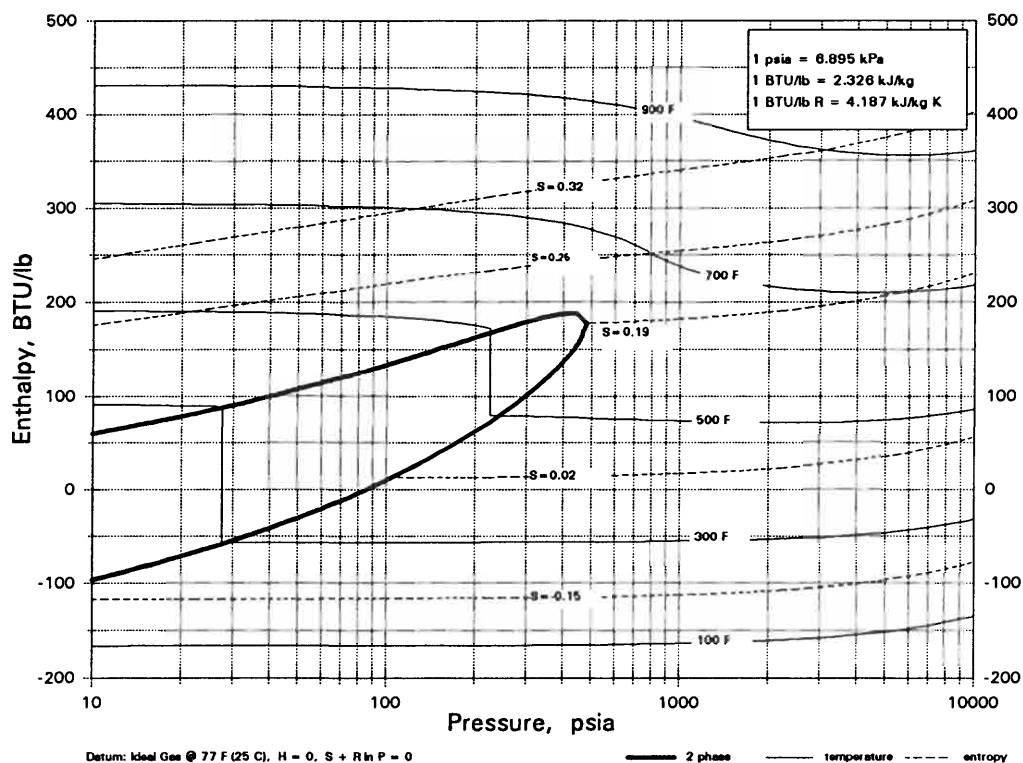
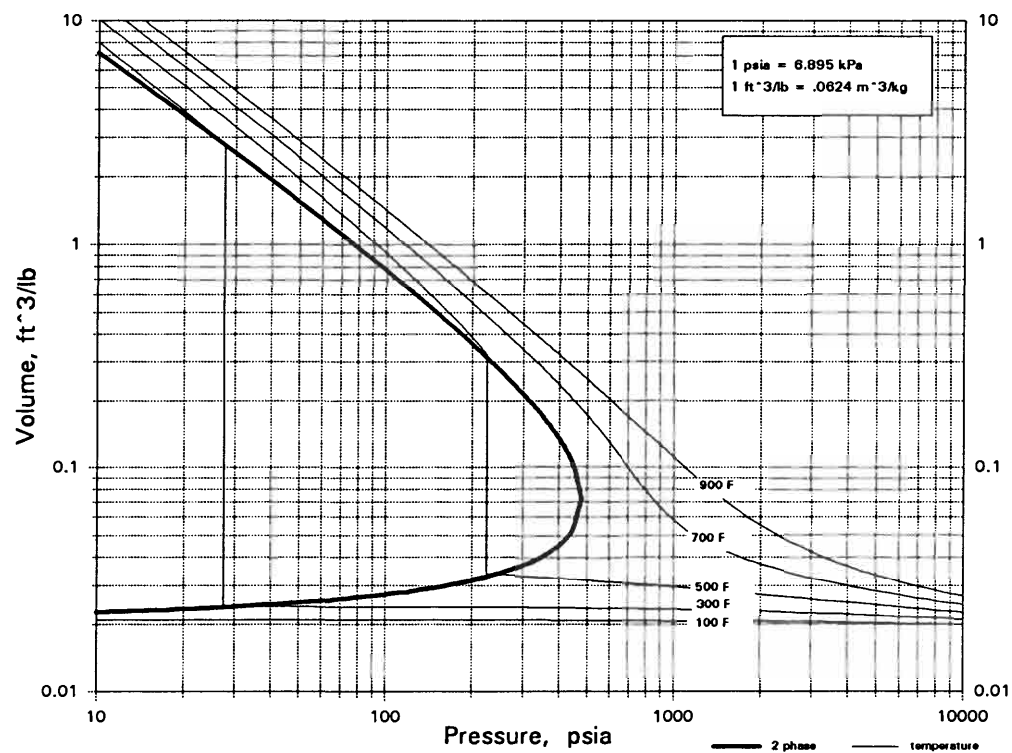
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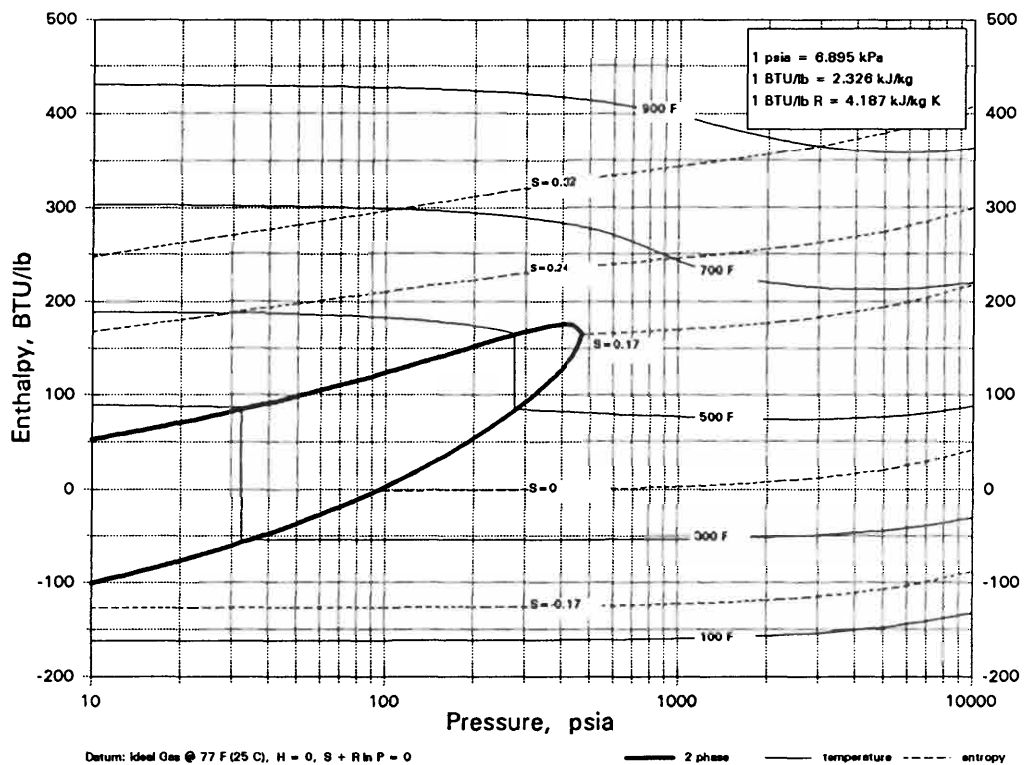
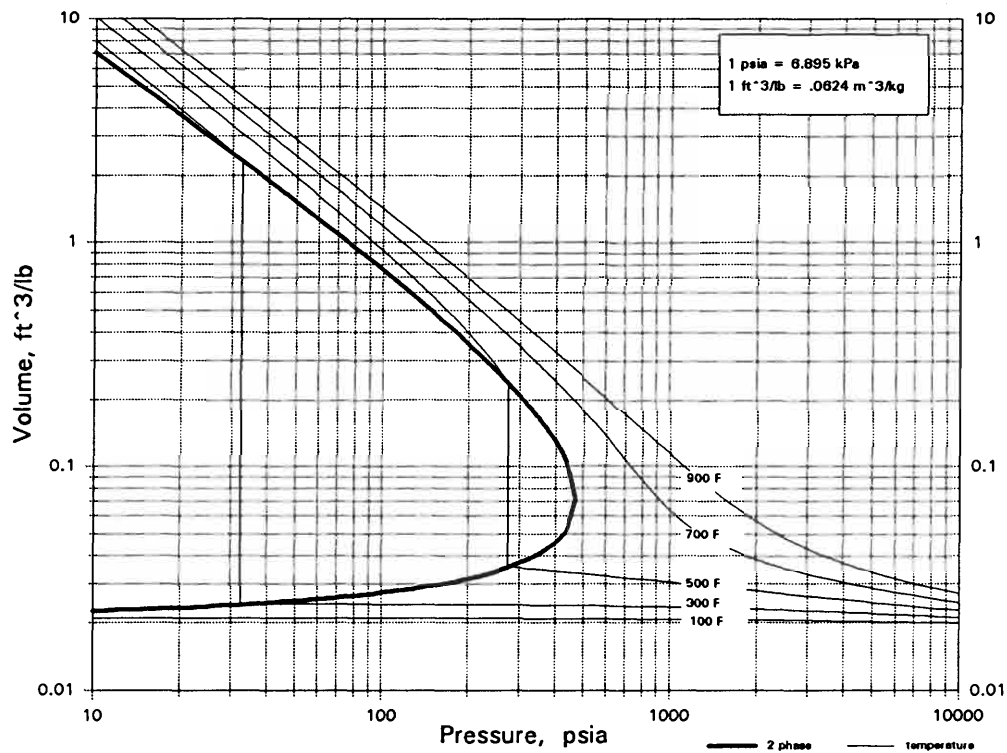
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3-HEXANONE



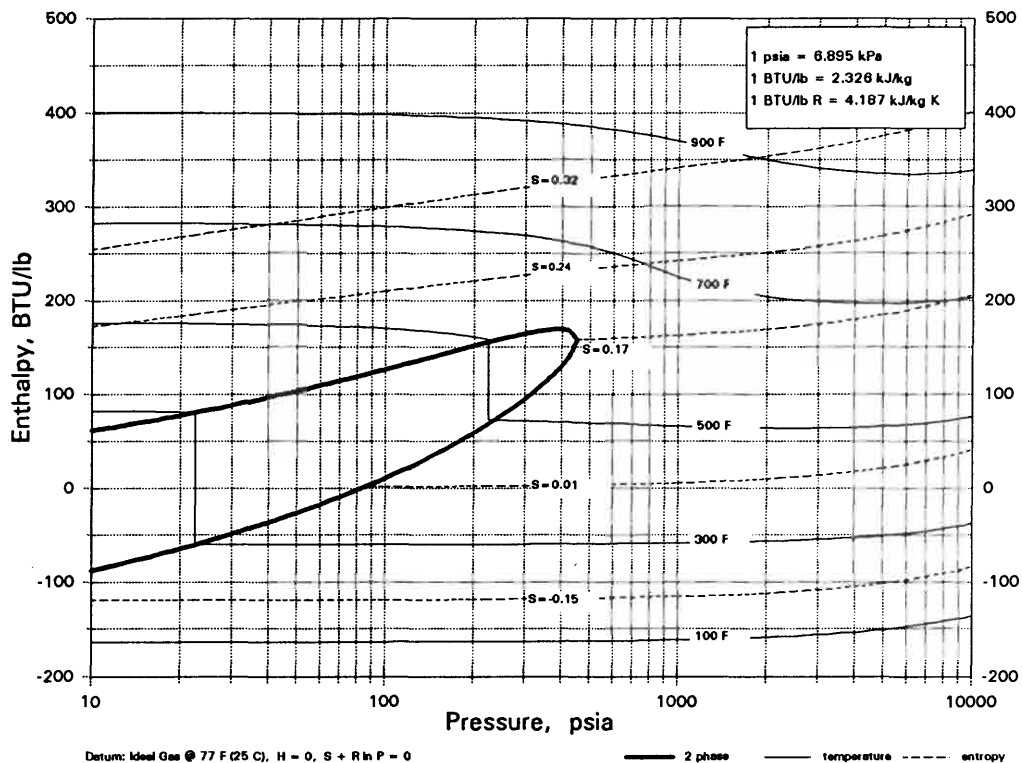
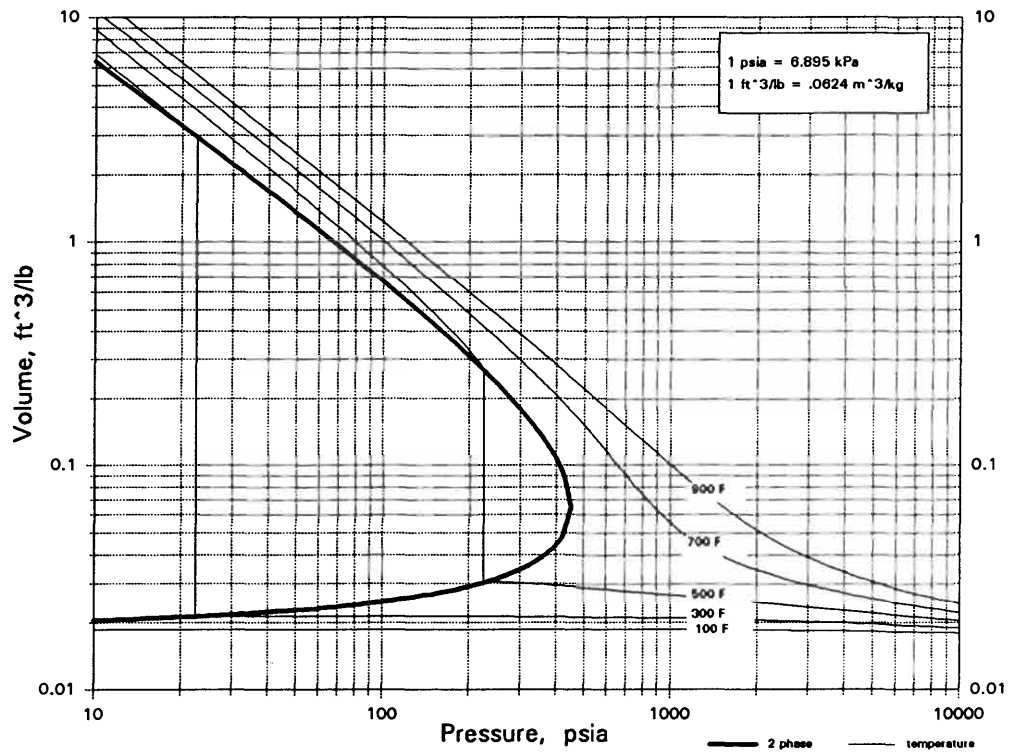
C6H12O

METHYL ISOBUTYL KETONE



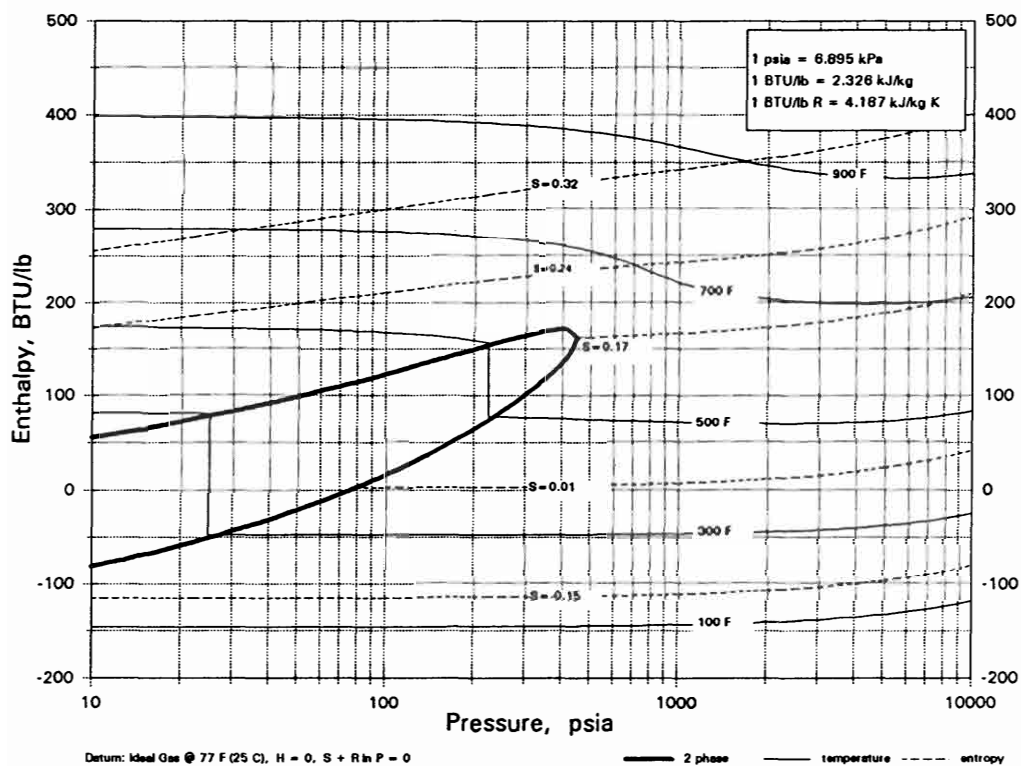
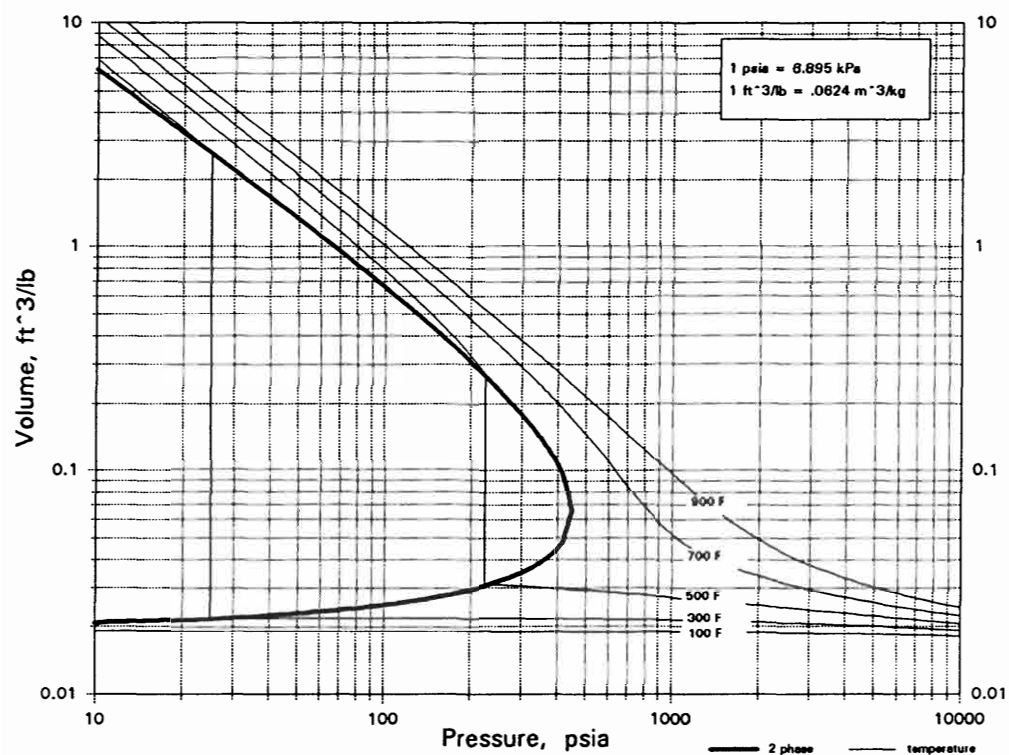
C6H12O2

n-PENTYL FORMATE



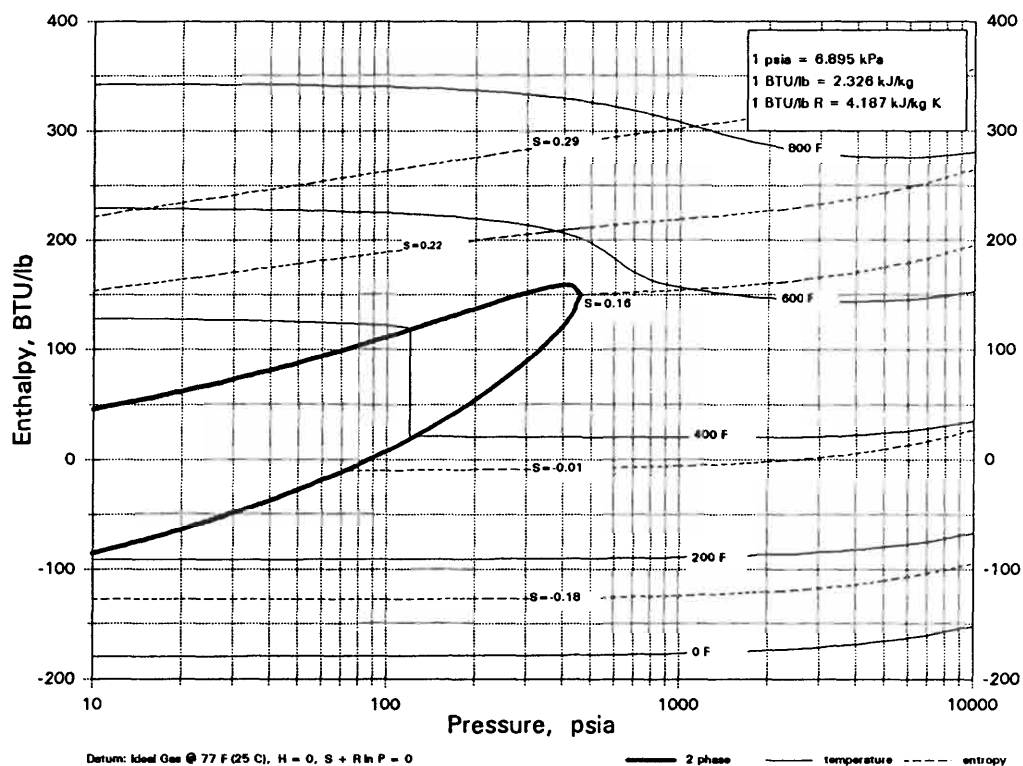
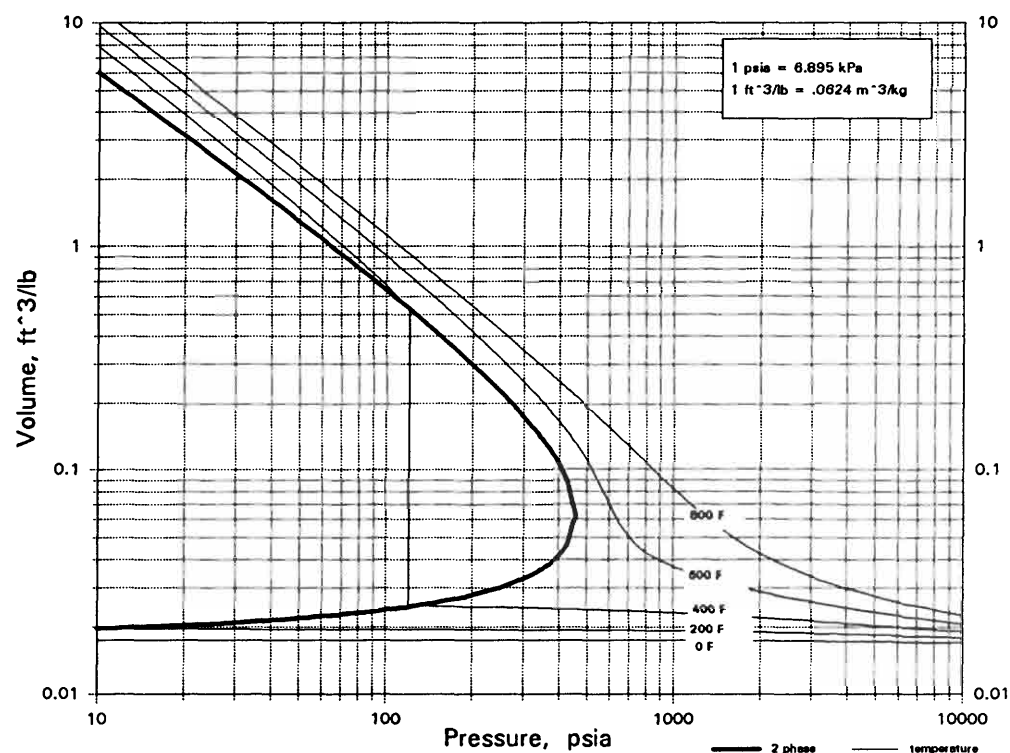
C6H12O2

n-BUTYL ACETATE



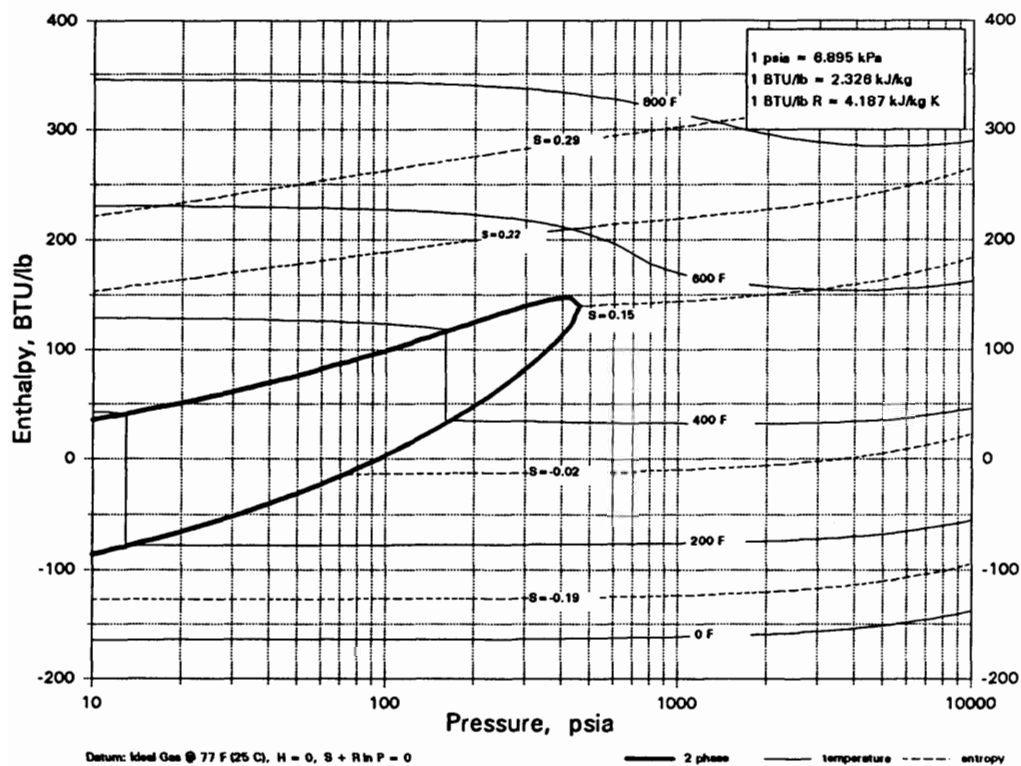
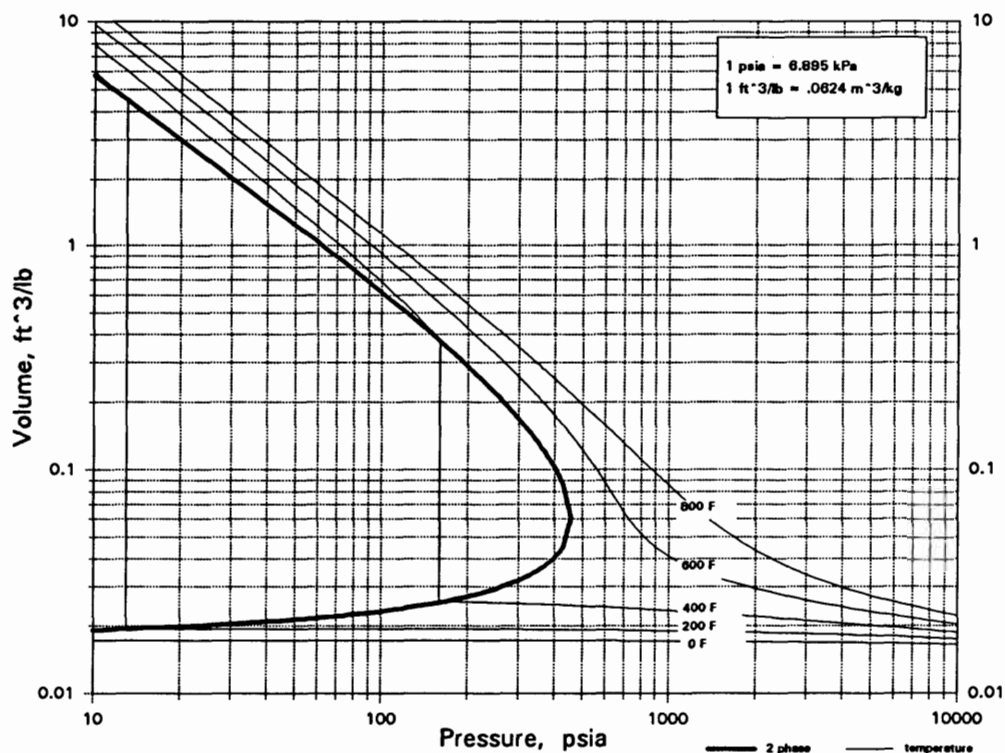
C6H12O2

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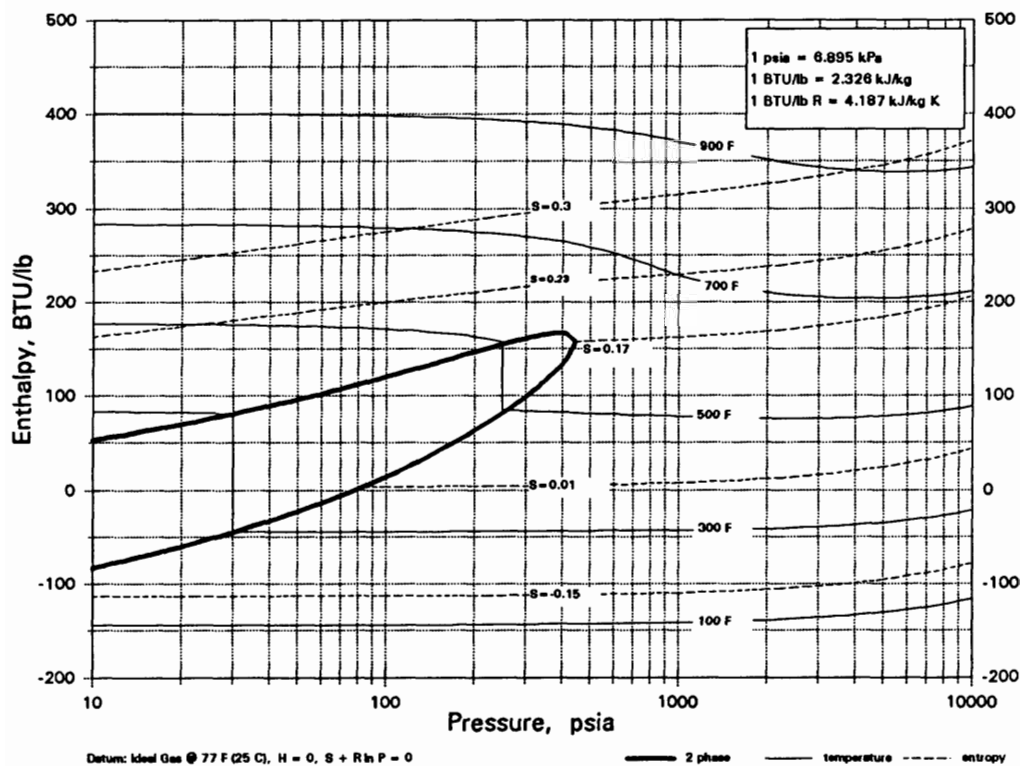
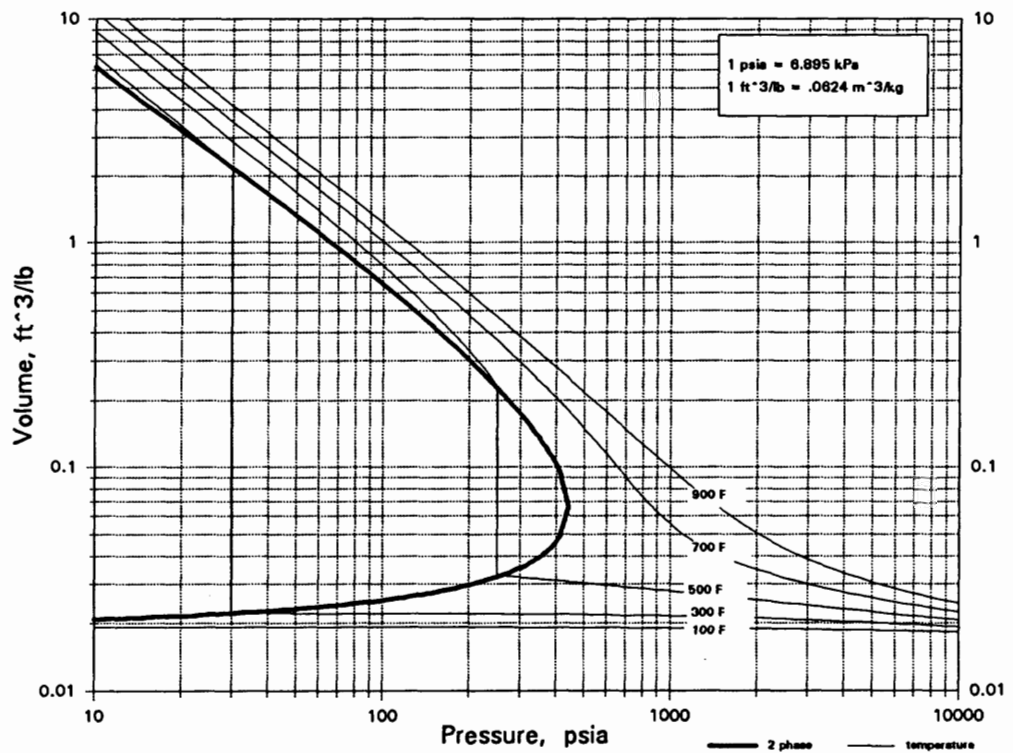


C6H12O2

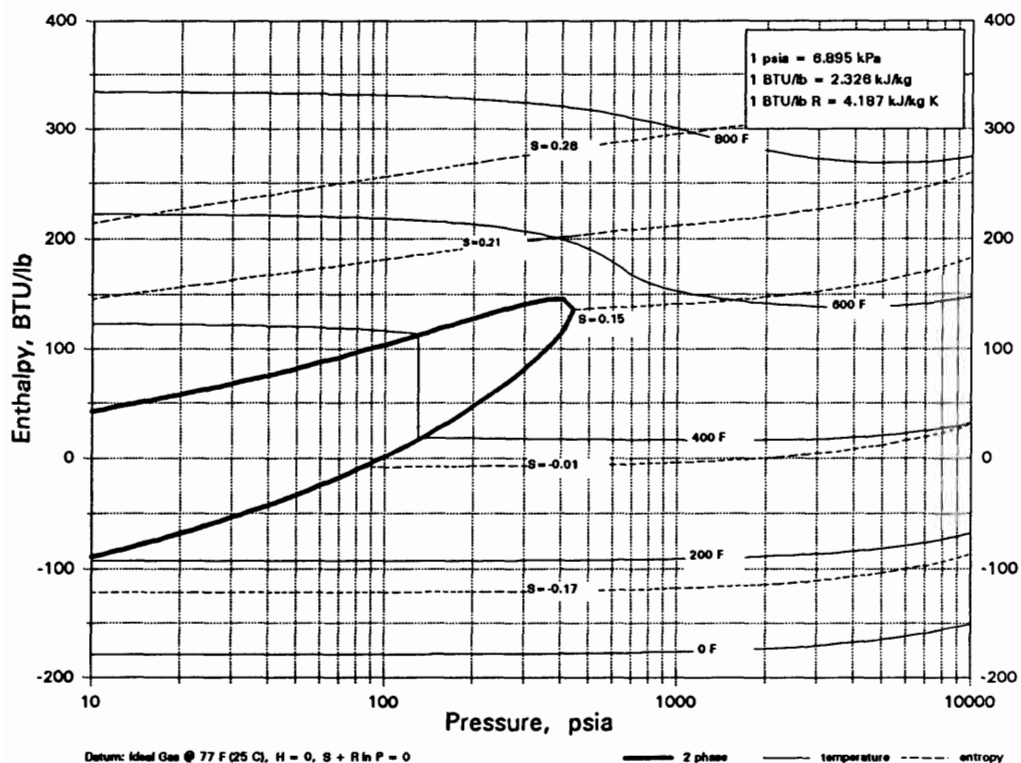
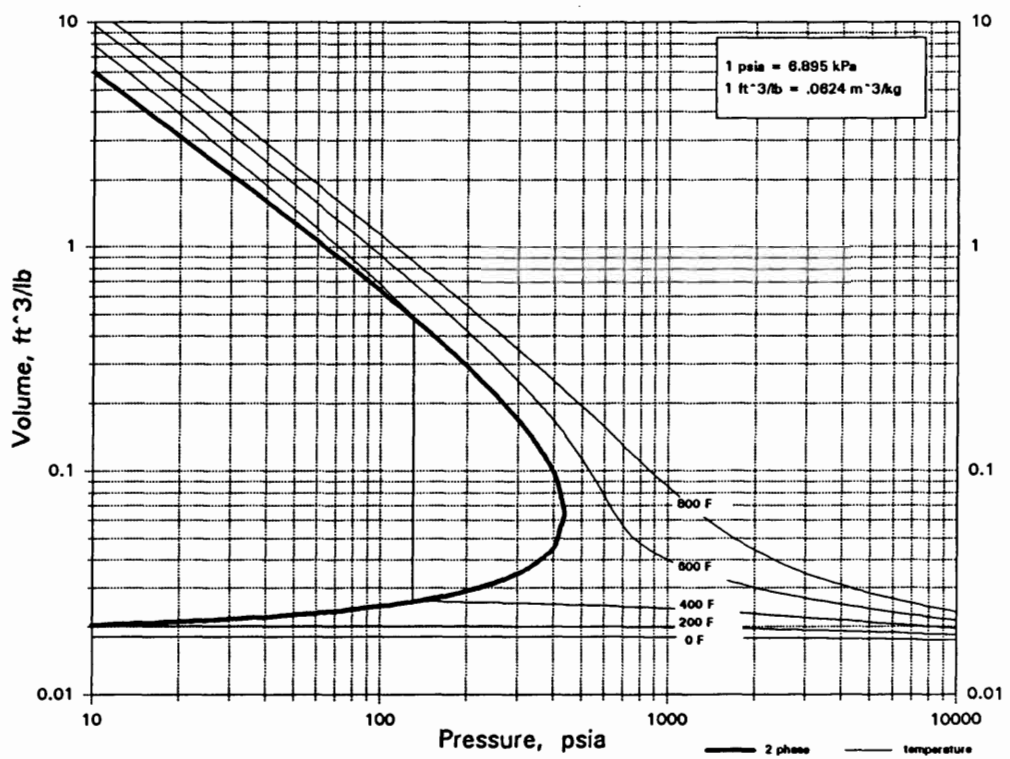
tert-BUTYL ACETATE



C6H12O2
ETHYL n-BUTYRATE

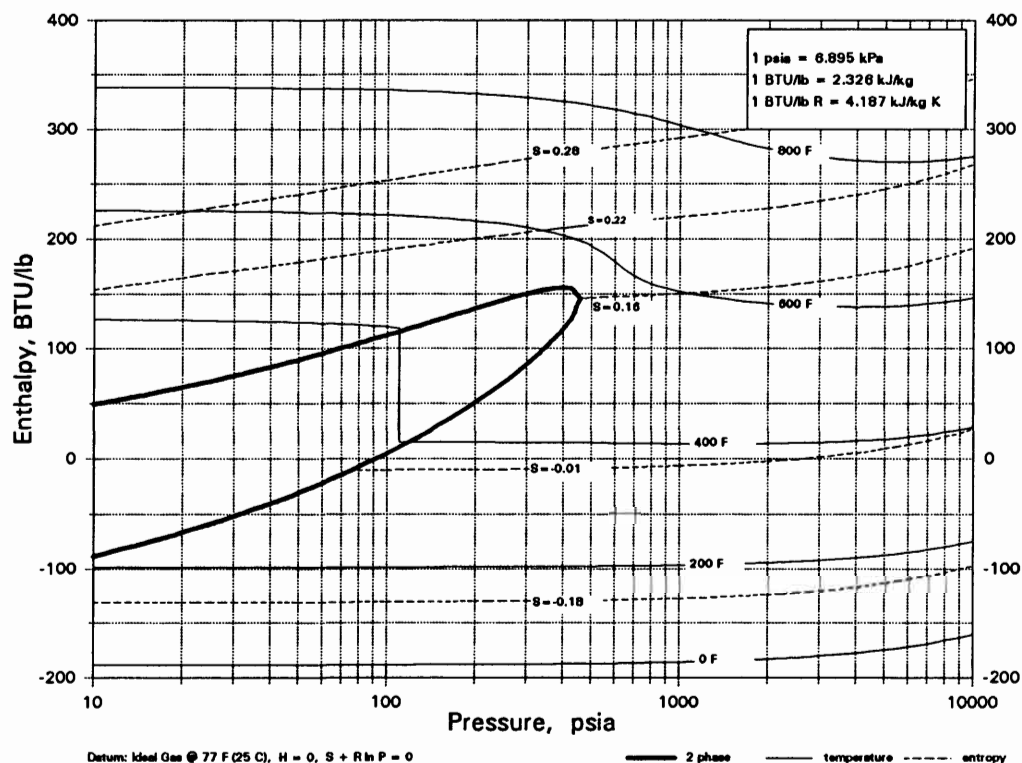
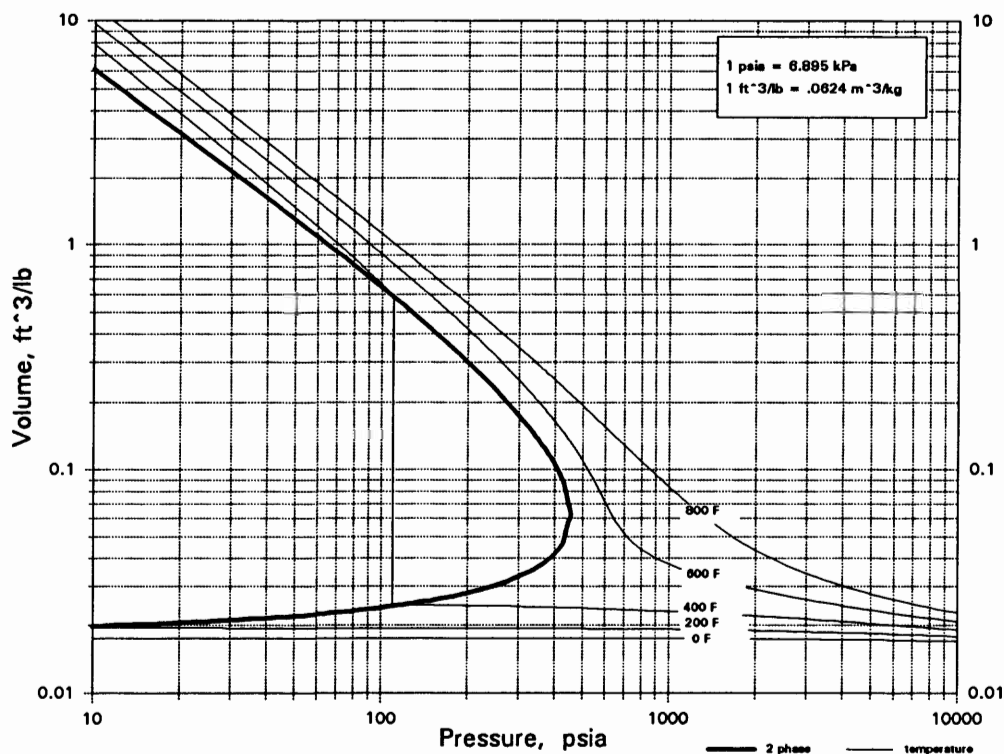


C6H12O2
ETHYL ISOBUTYRATE



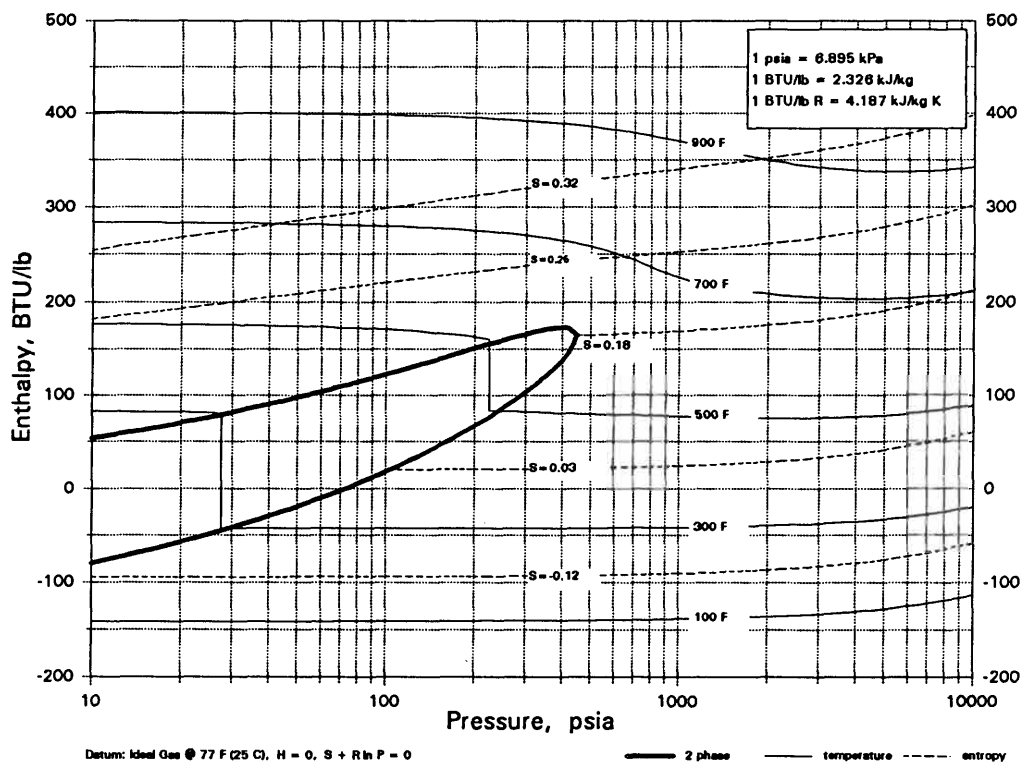
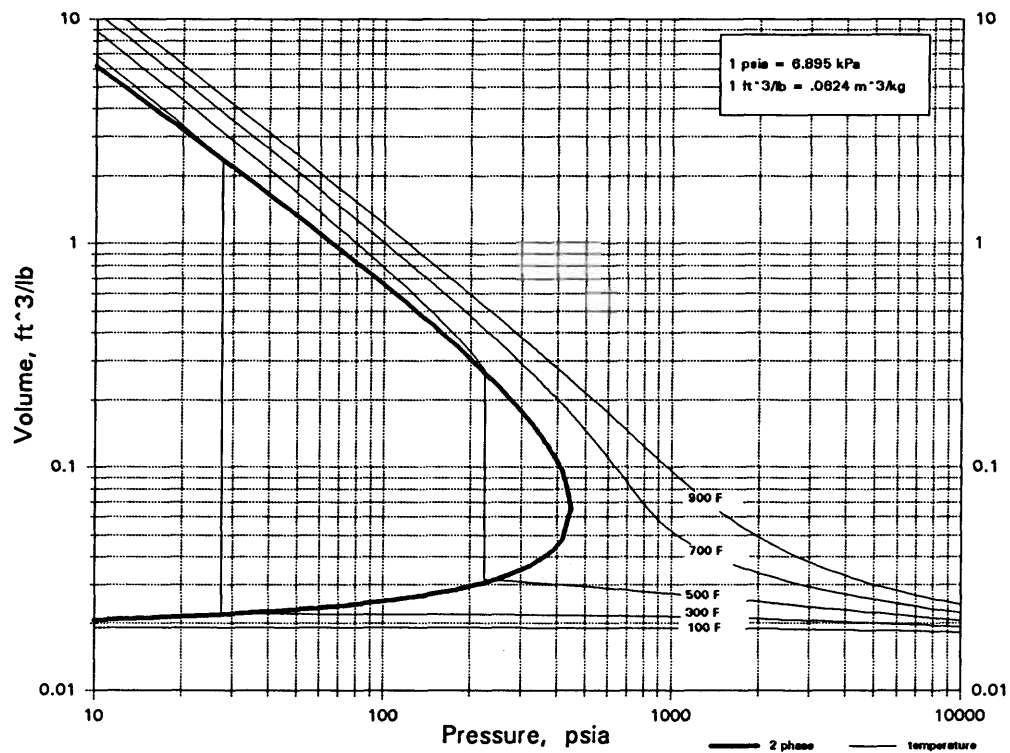
C6H12O2

ISOBUTYL ACETATE



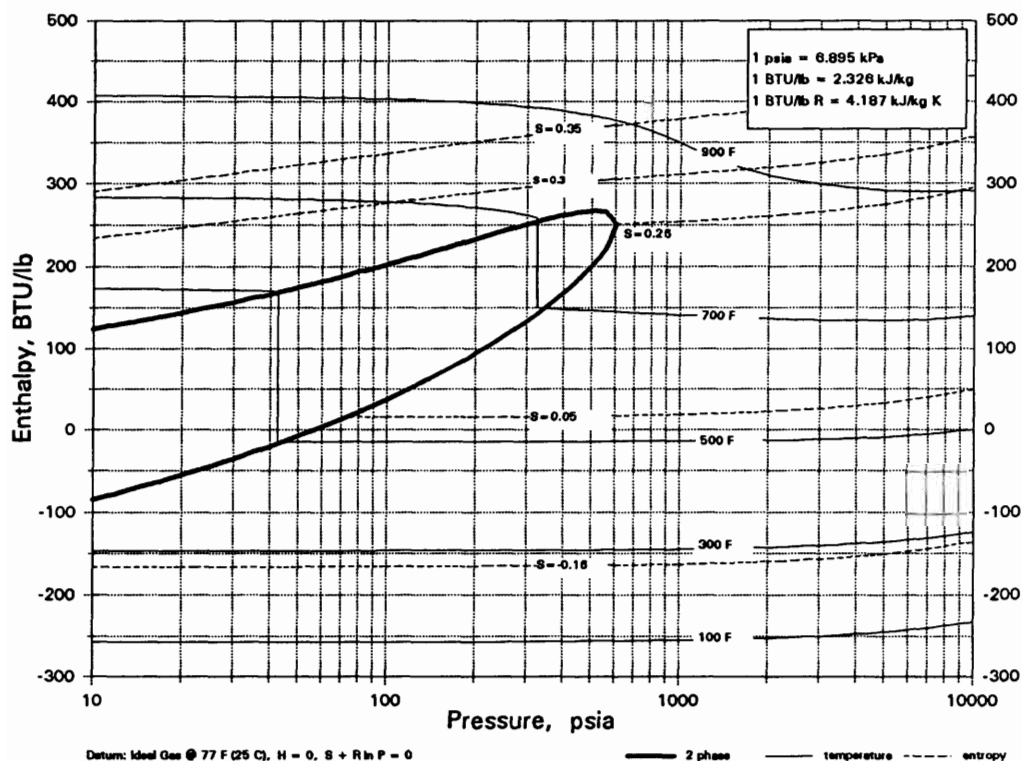
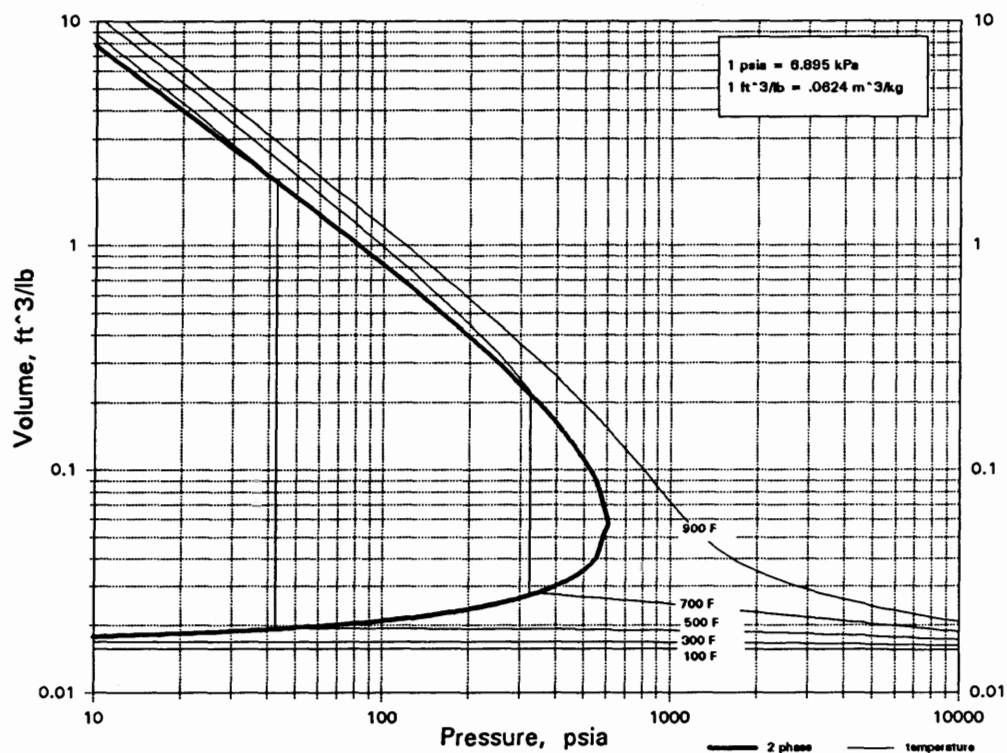
C6H12O2

n-PROPYL PROPIONATE



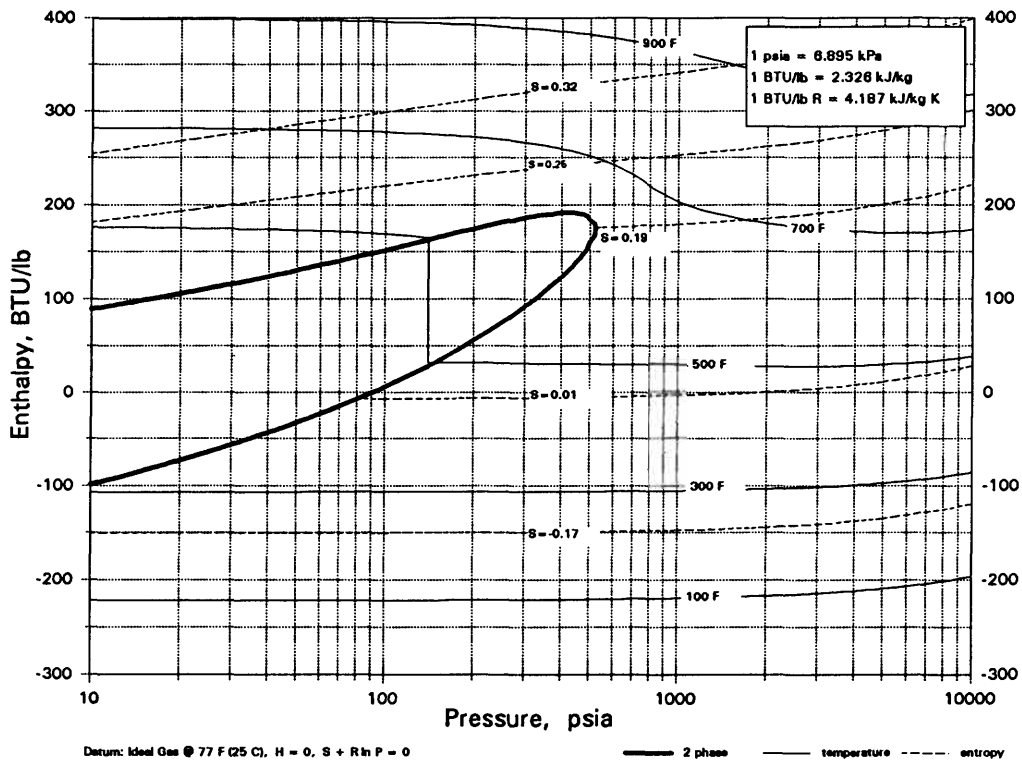
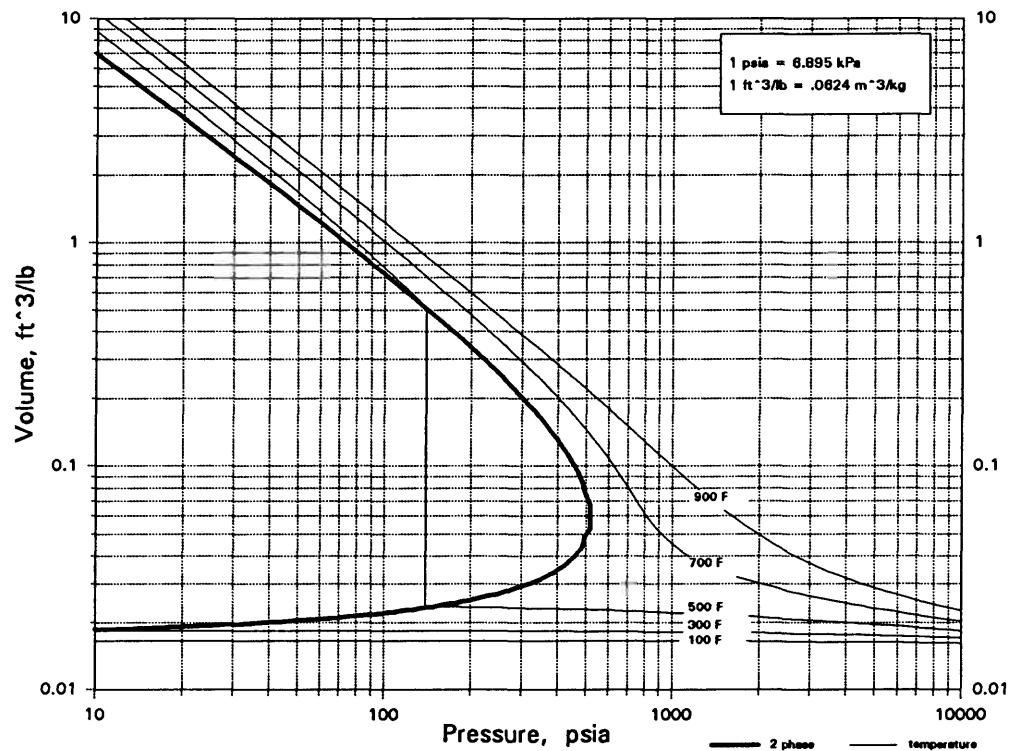
C6H12O2

CYCLOHEXYL PEROXIDE



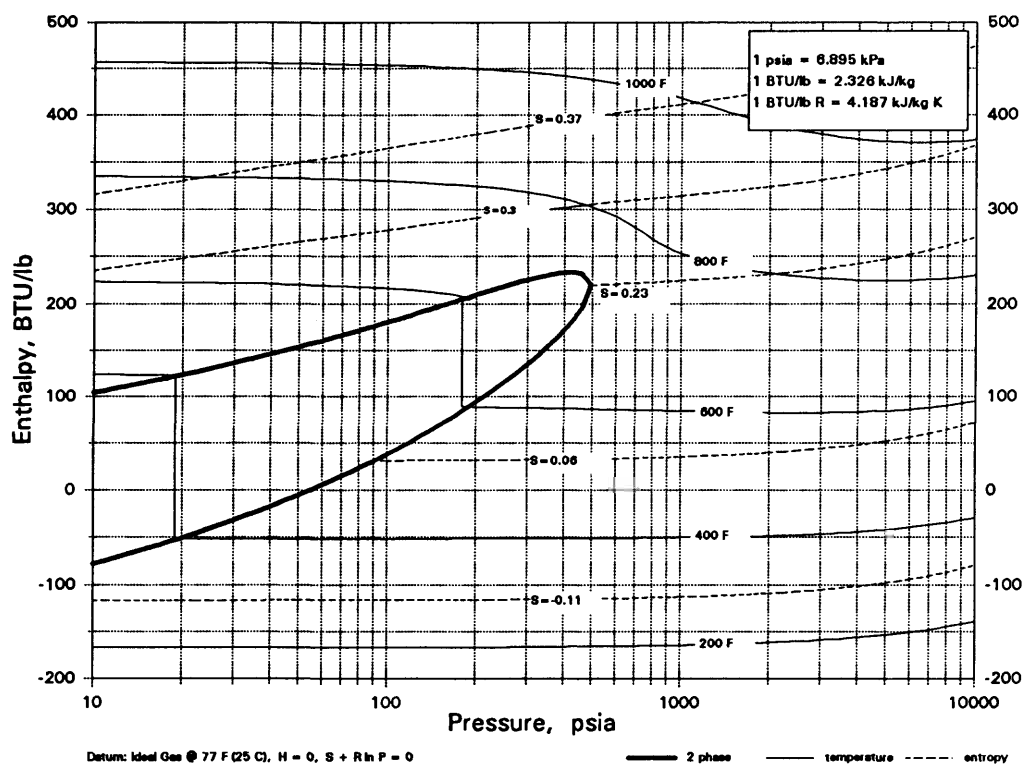
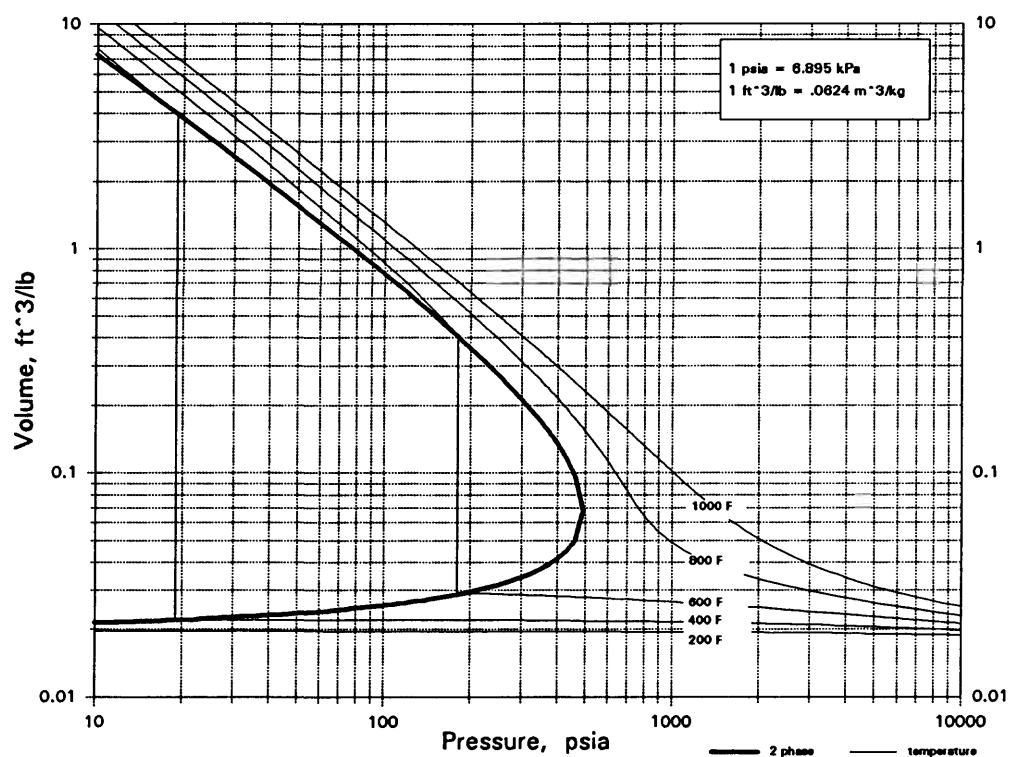
C6H12O2

DIACETONE ALCOHOL



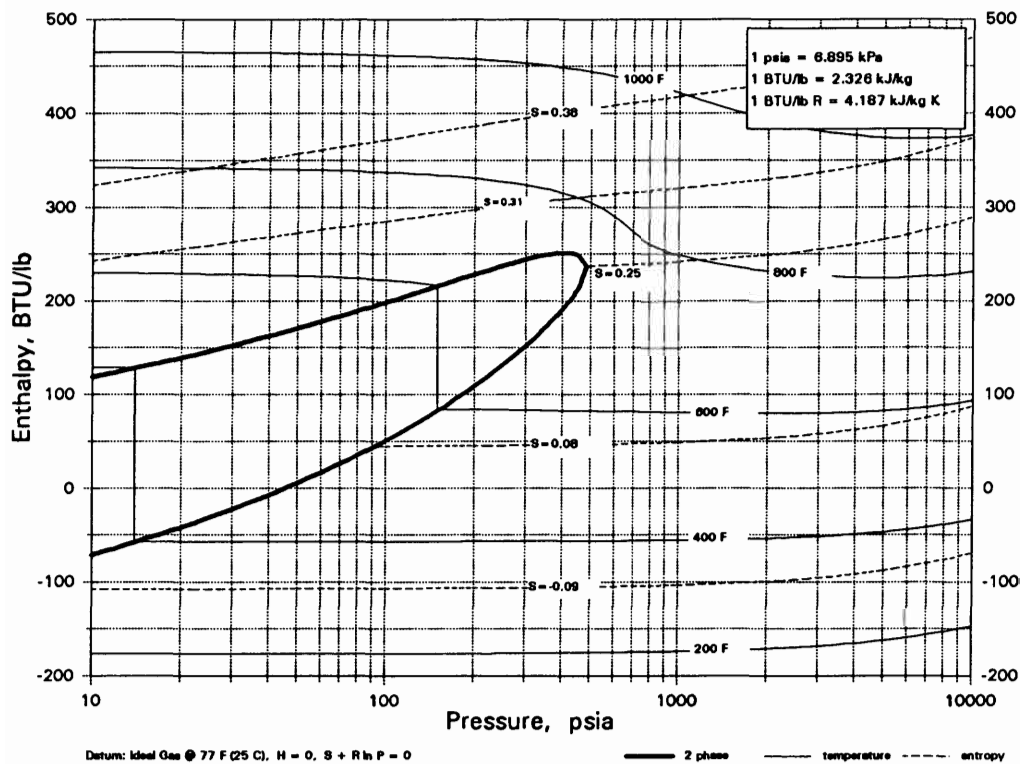
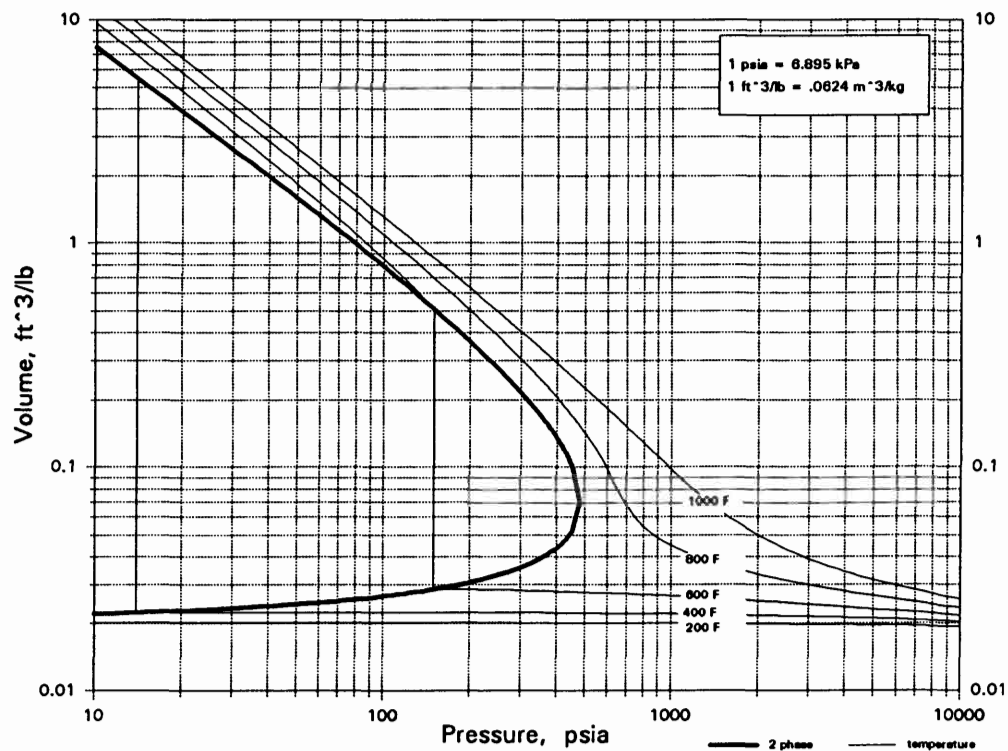
C6H12O2

2-ETHYL BUTYRIC ACID



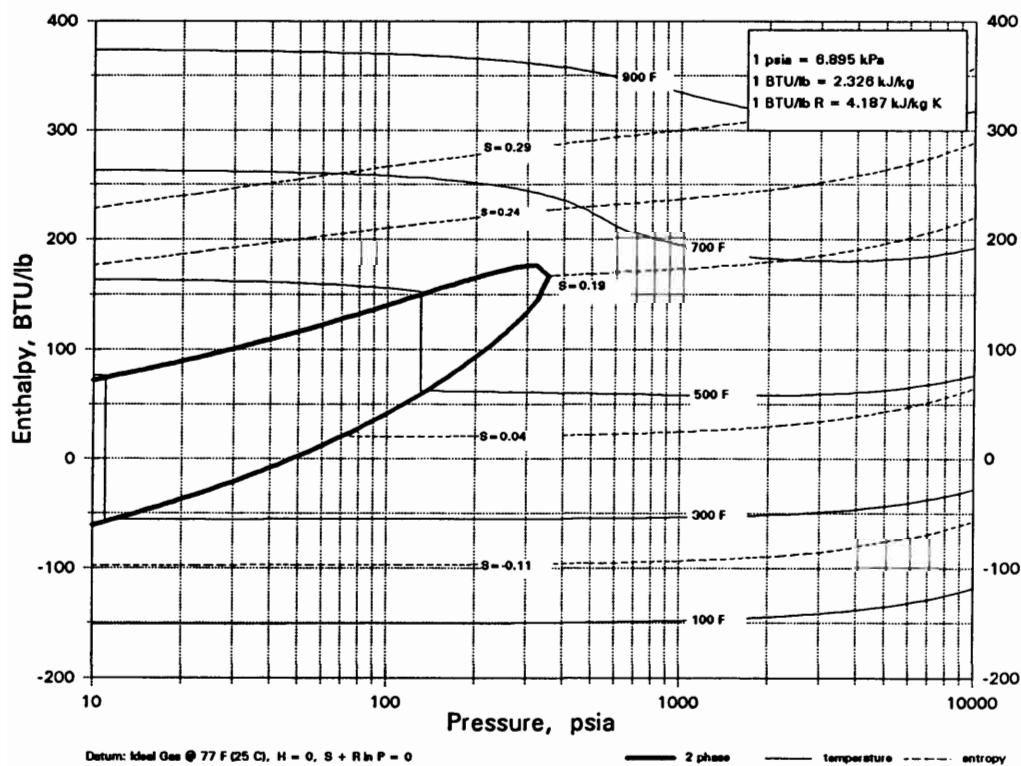
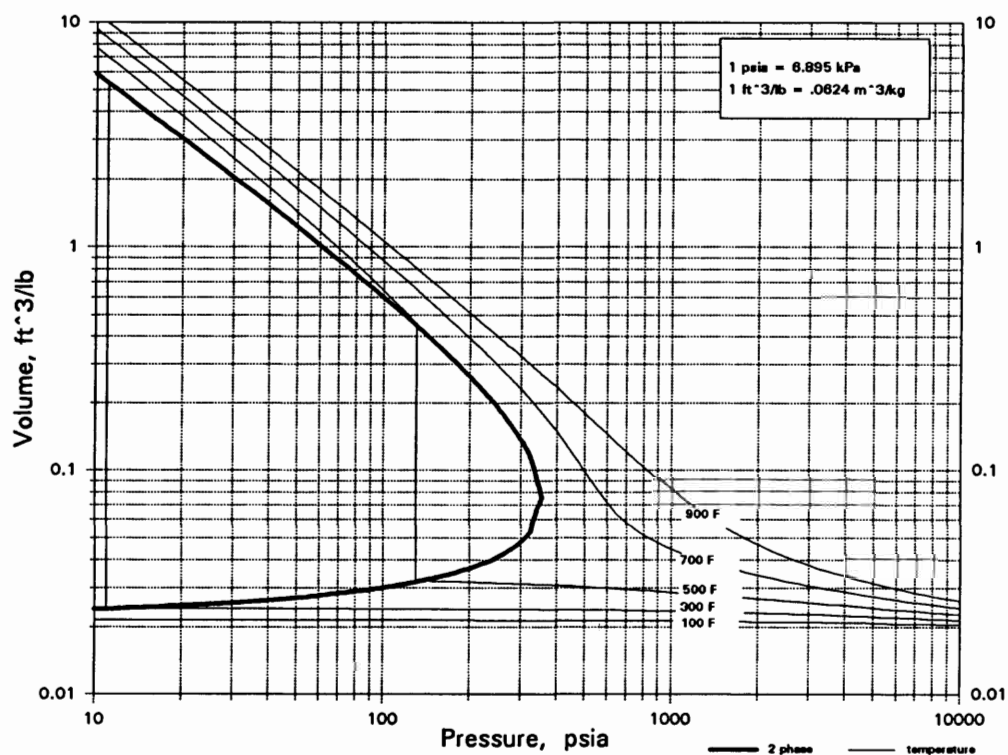
C6H12O2

n-HEXANOIC ACID



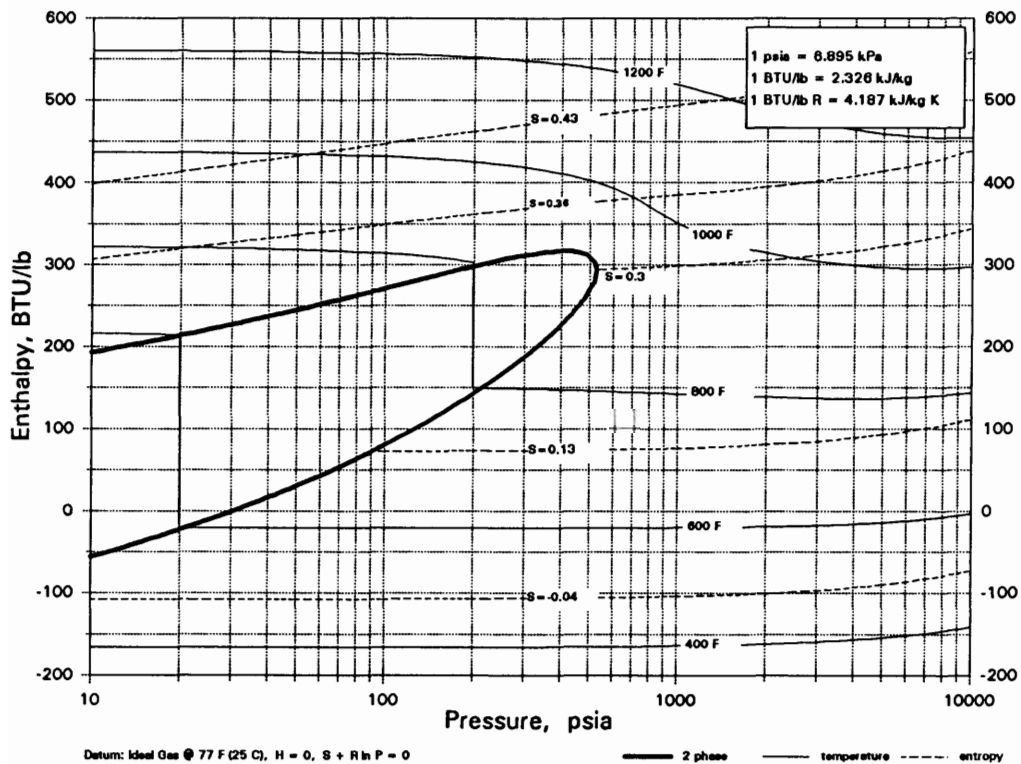
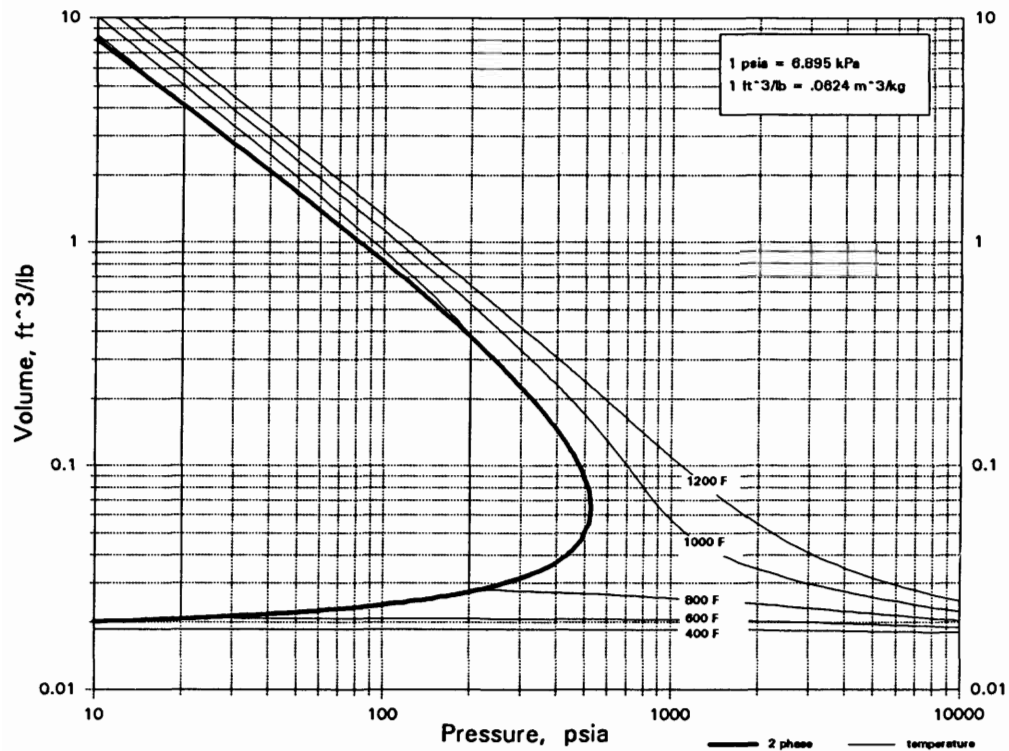
C6H12O3

2-ETHOXYETHYL ACETATE



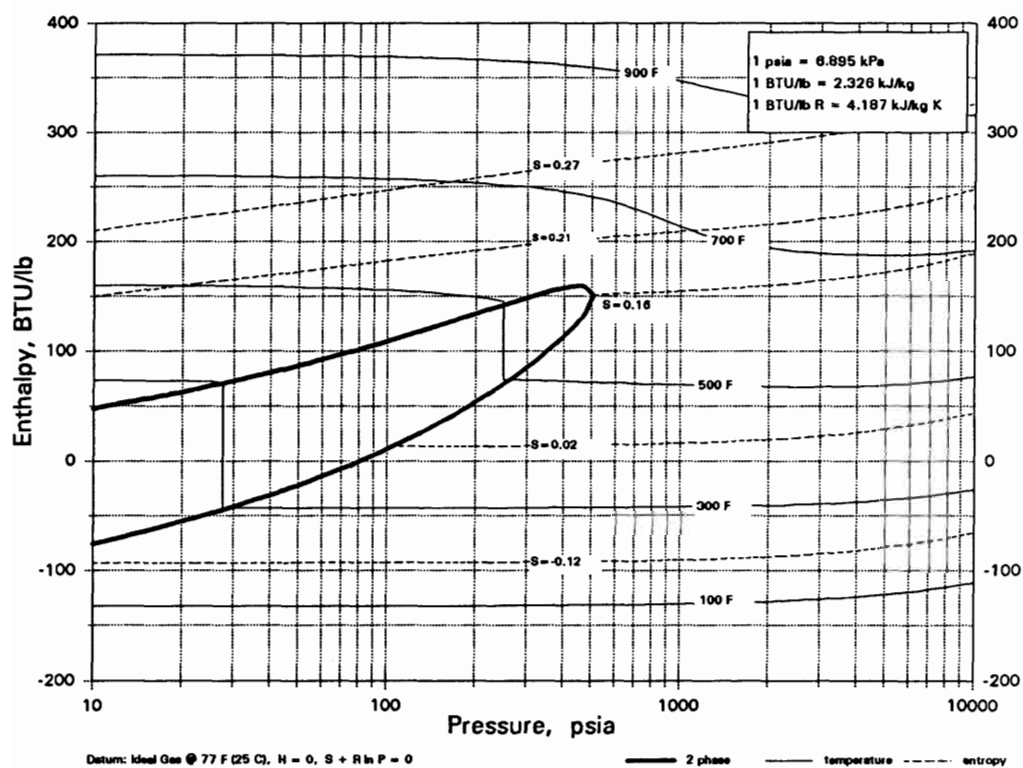
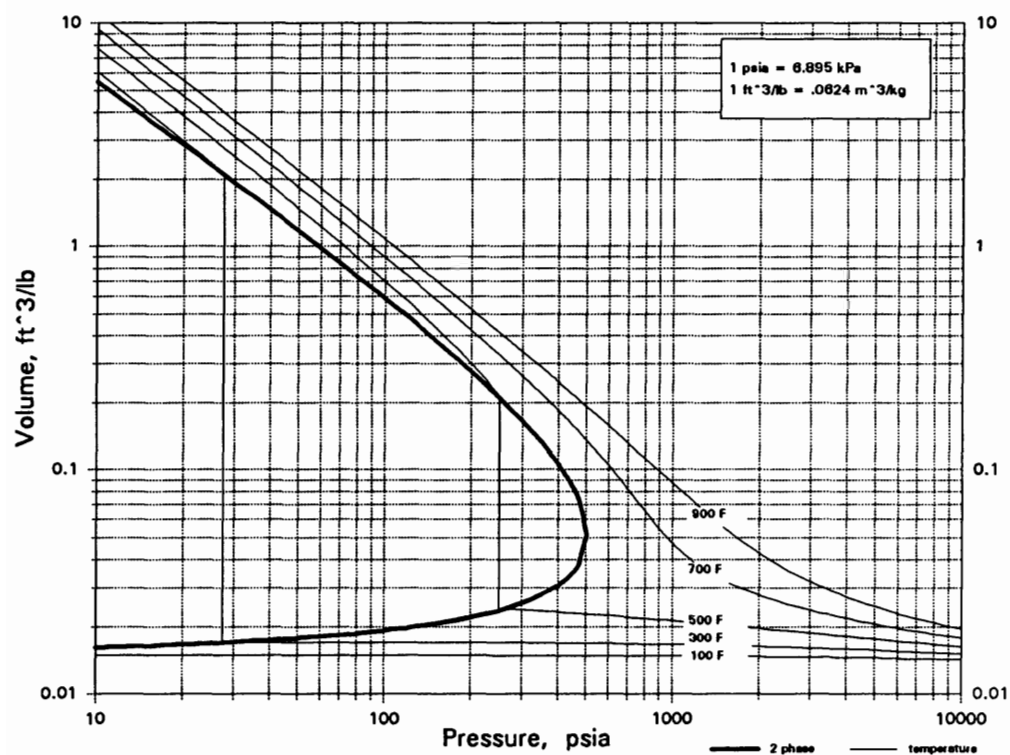
C6H12O3

HYDROXYCAPROIC ACID



C6H12O3

PARALDEHYDE



C6H12O3

sec-BUTYL GLYCOLATE

1. Molecular Weight, lb/mol..... 132.16

2. Boiling Point, K..... 450.65

Critical data (Tc, Pc) are not available.

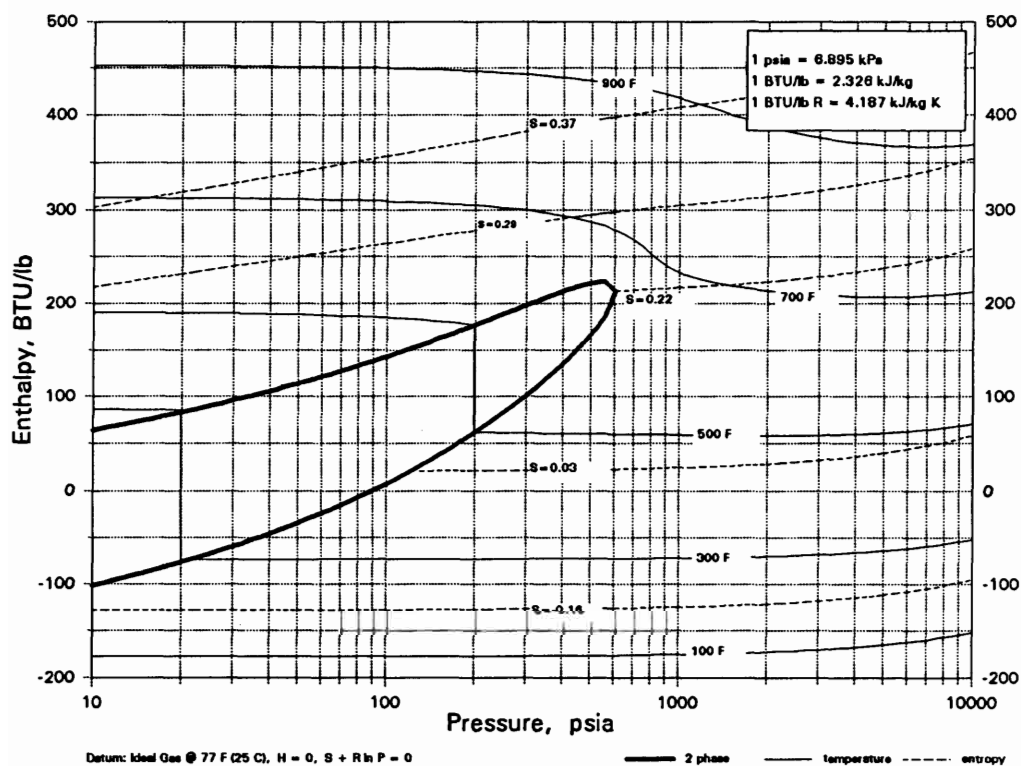
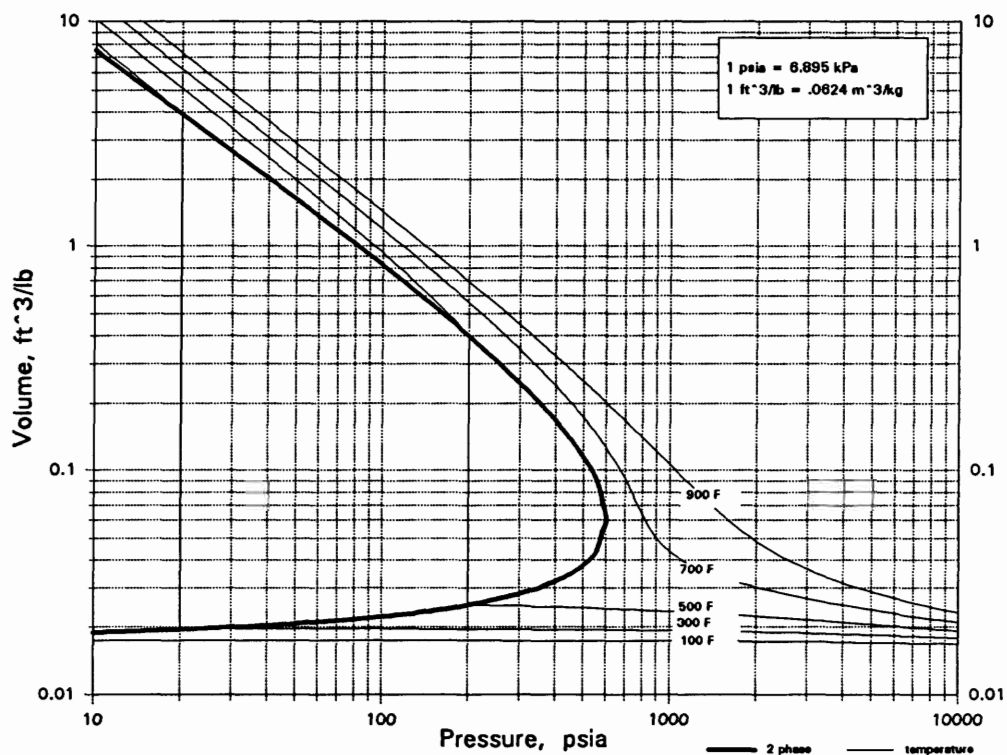
1. Molecular Weight, lb/mol..... 132.16

2. Boiling Point, K..... 450.65

Critical data (Tc, Pc) are not available.

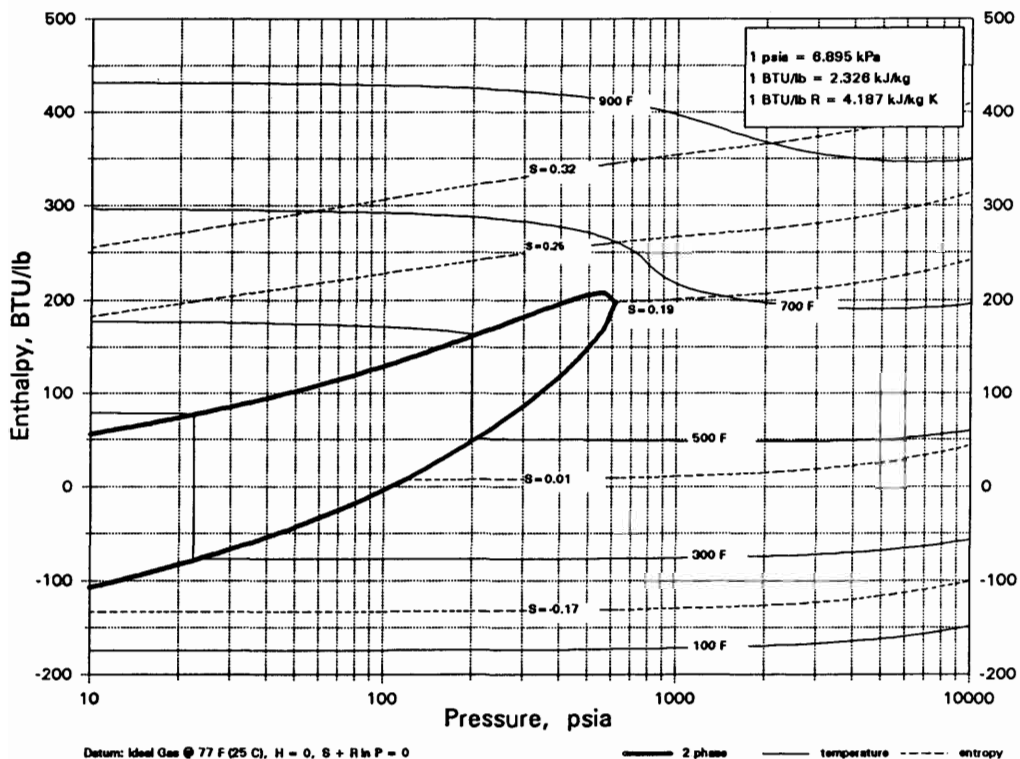
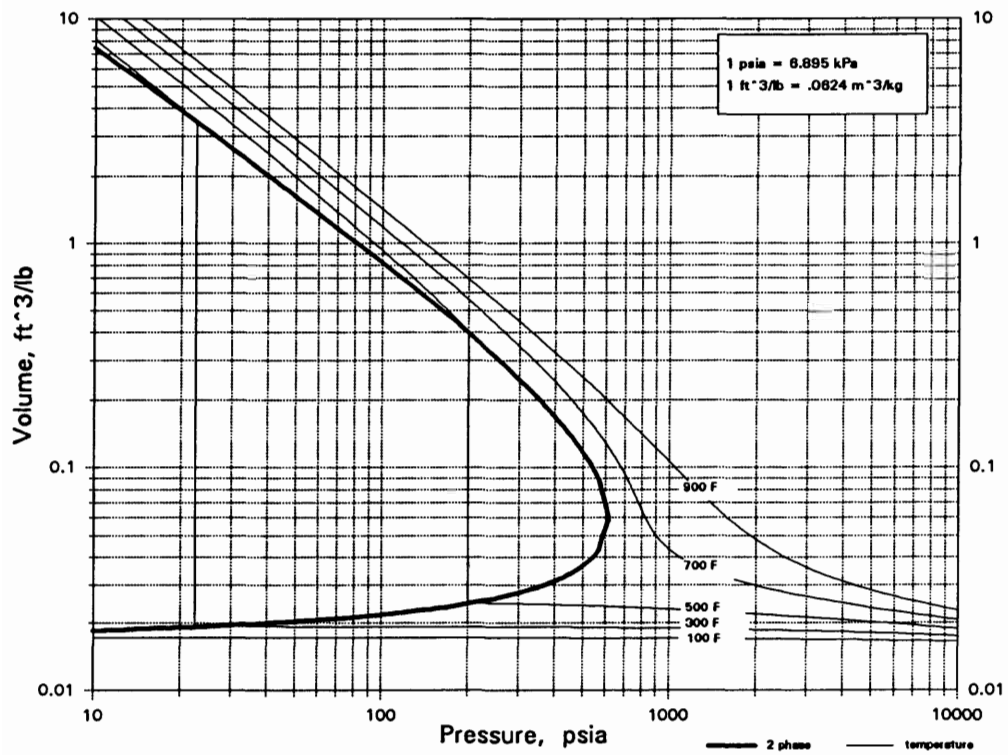
C6H13N

CYCLOHEXYLAMINE



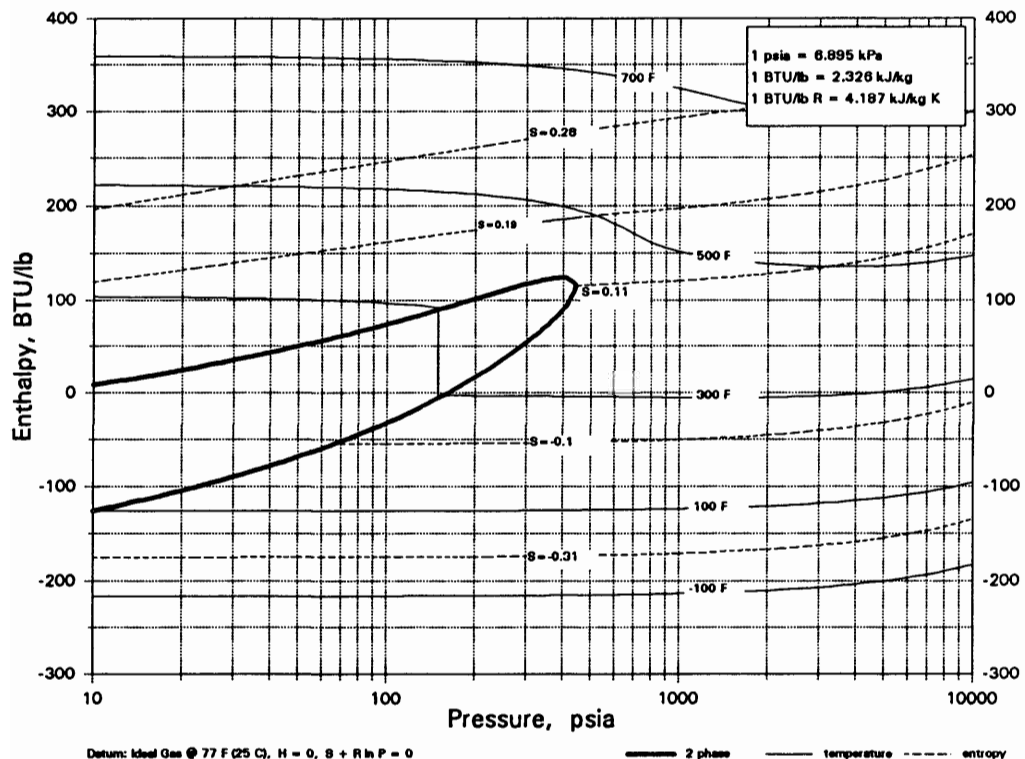
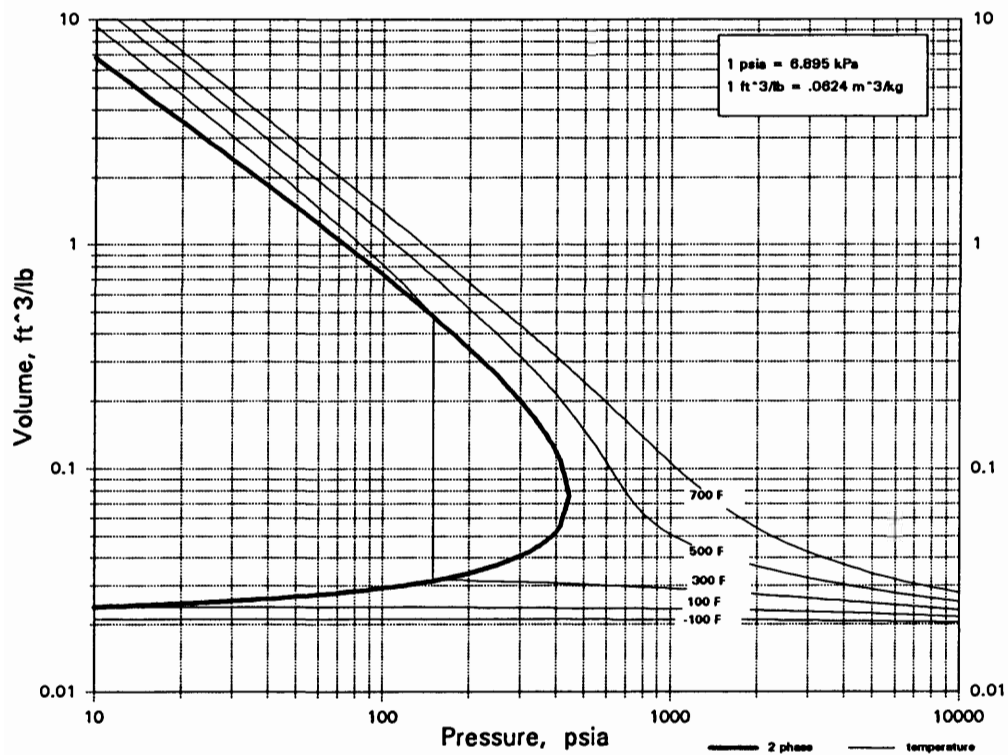
C6H13N

HEXAMETHYLENEIMINE



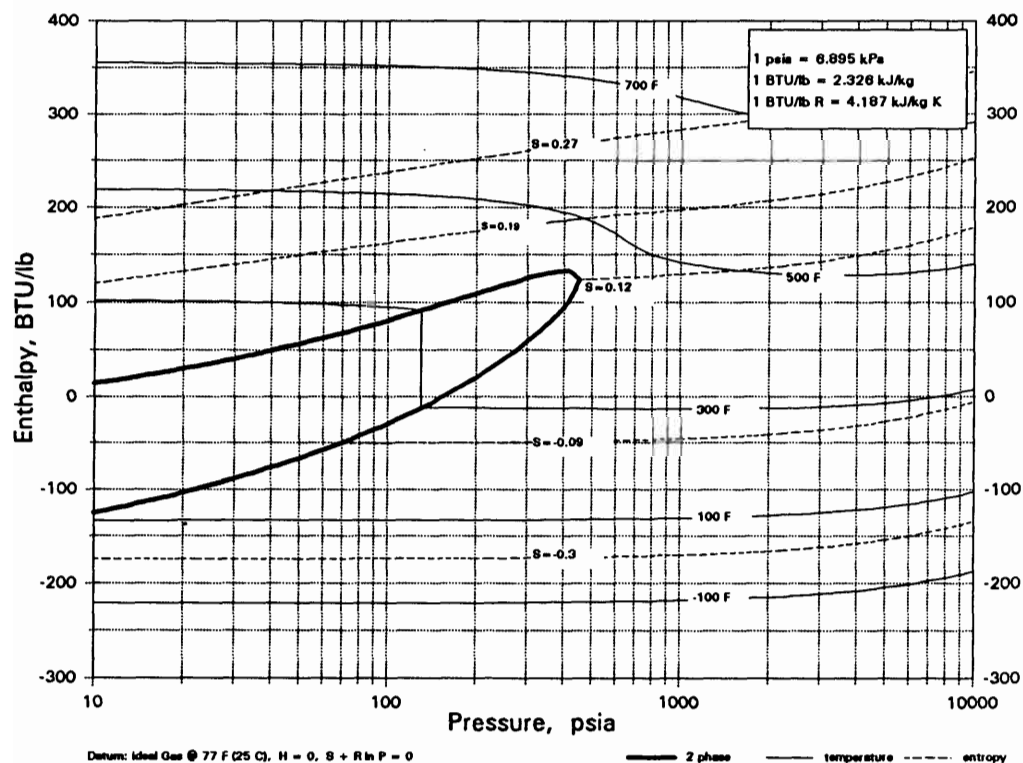
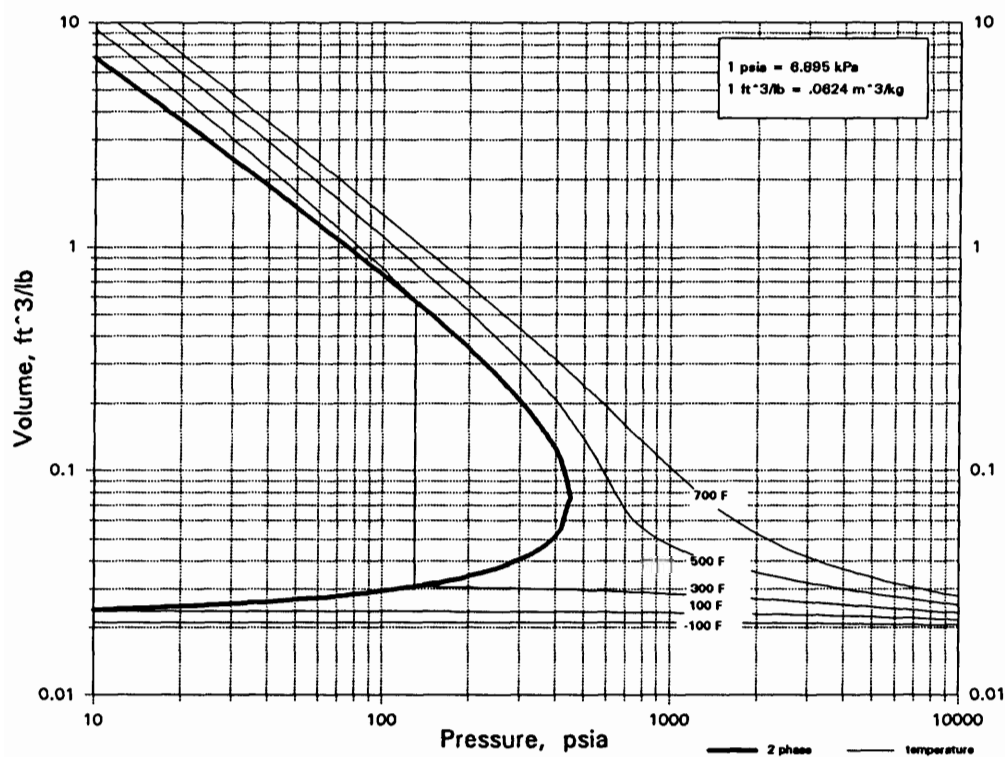
C6H14

2-2-DIMETHYLBUTANE



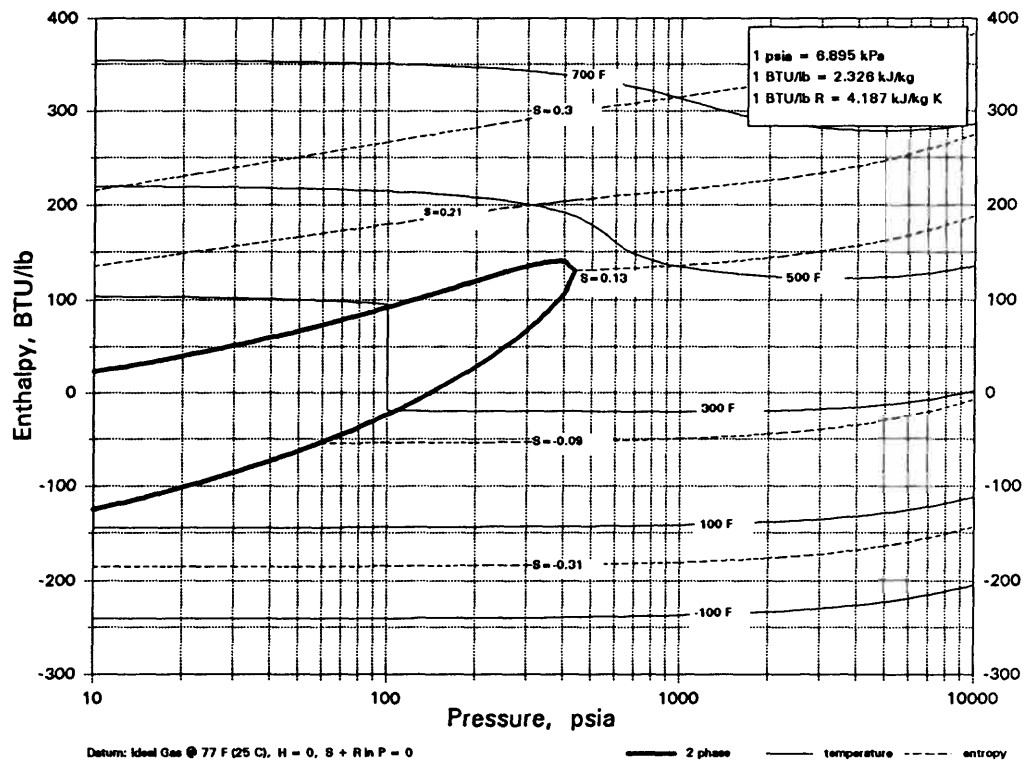
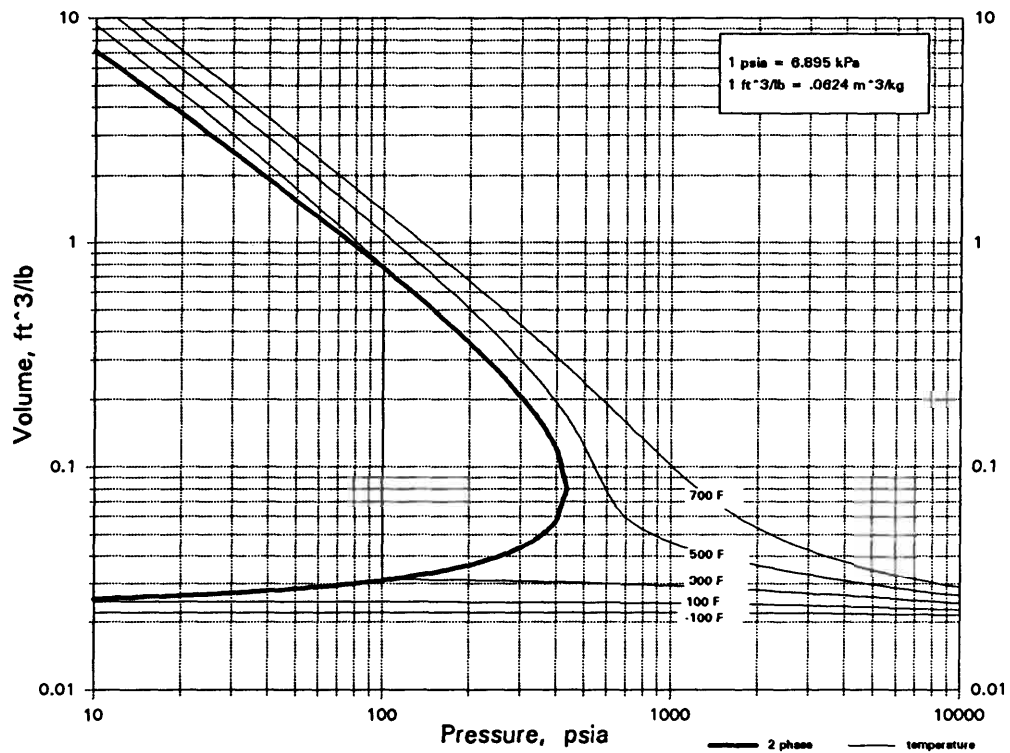
C6H14

2-3-DIMETHYLBUTANE



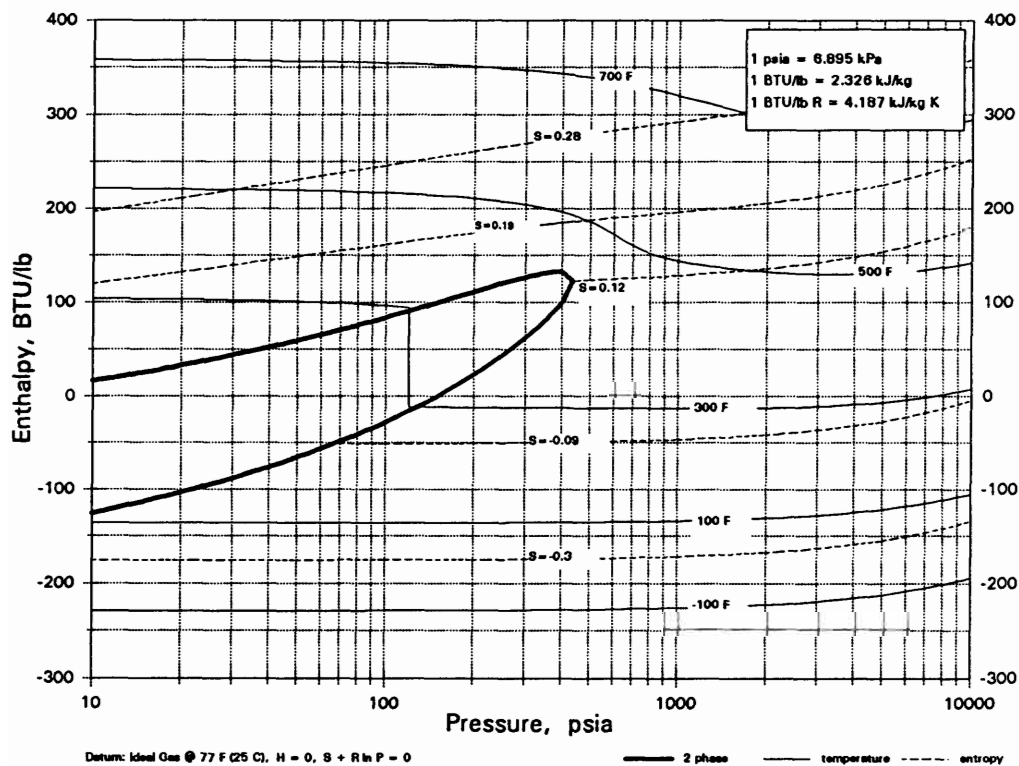
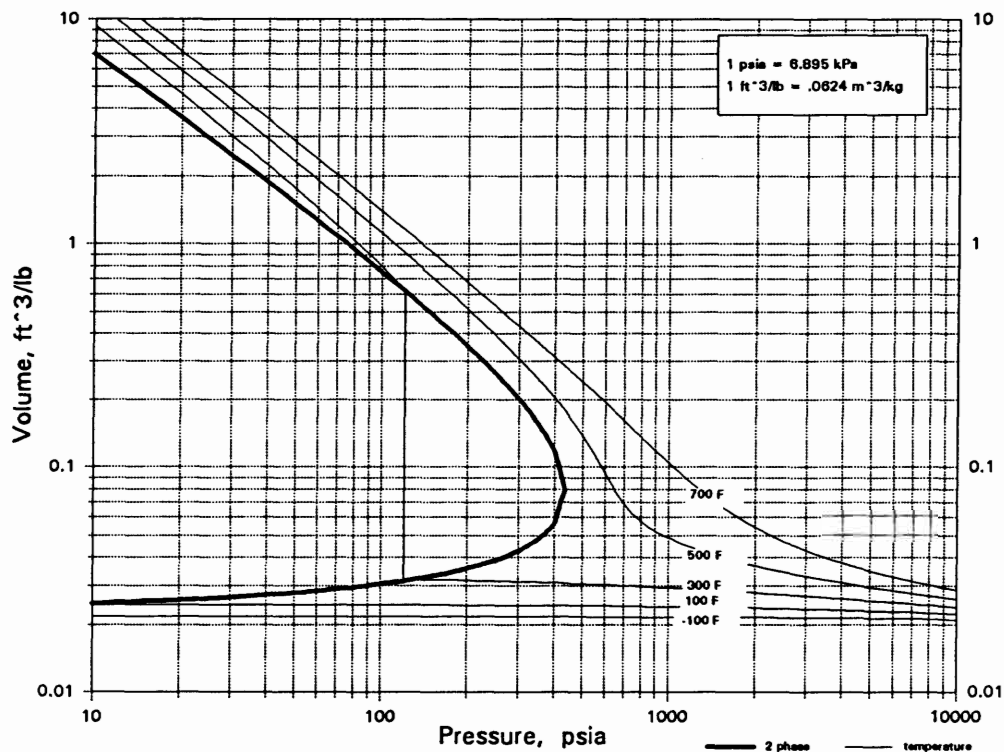
C6H14

n-HEXANE



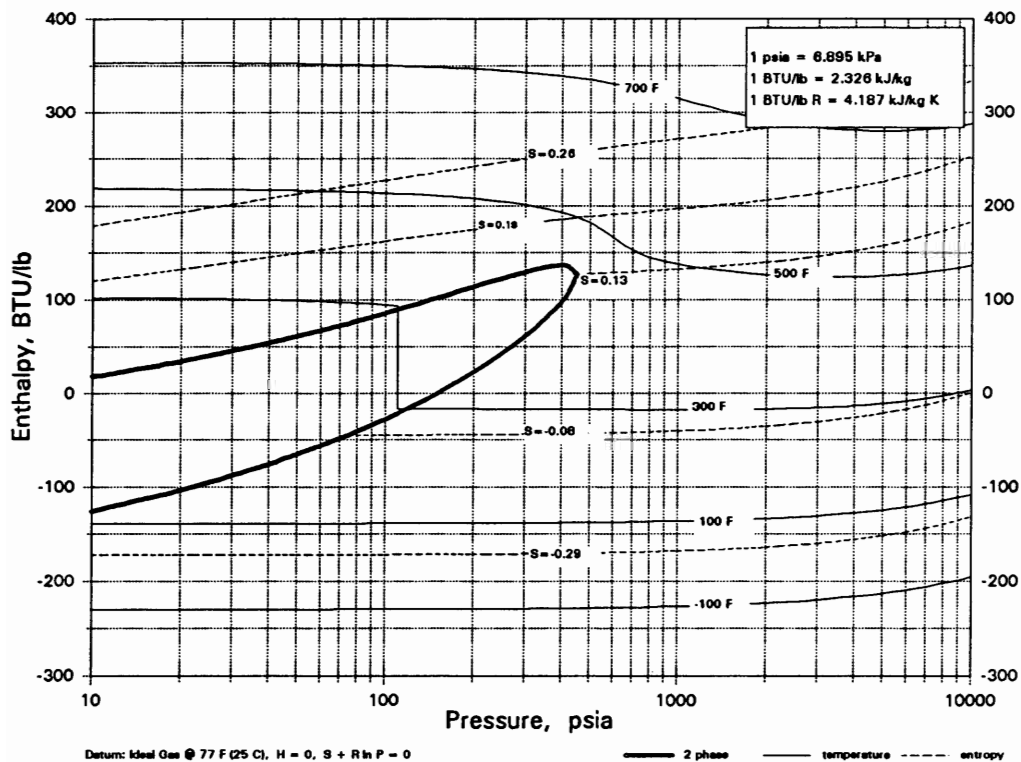
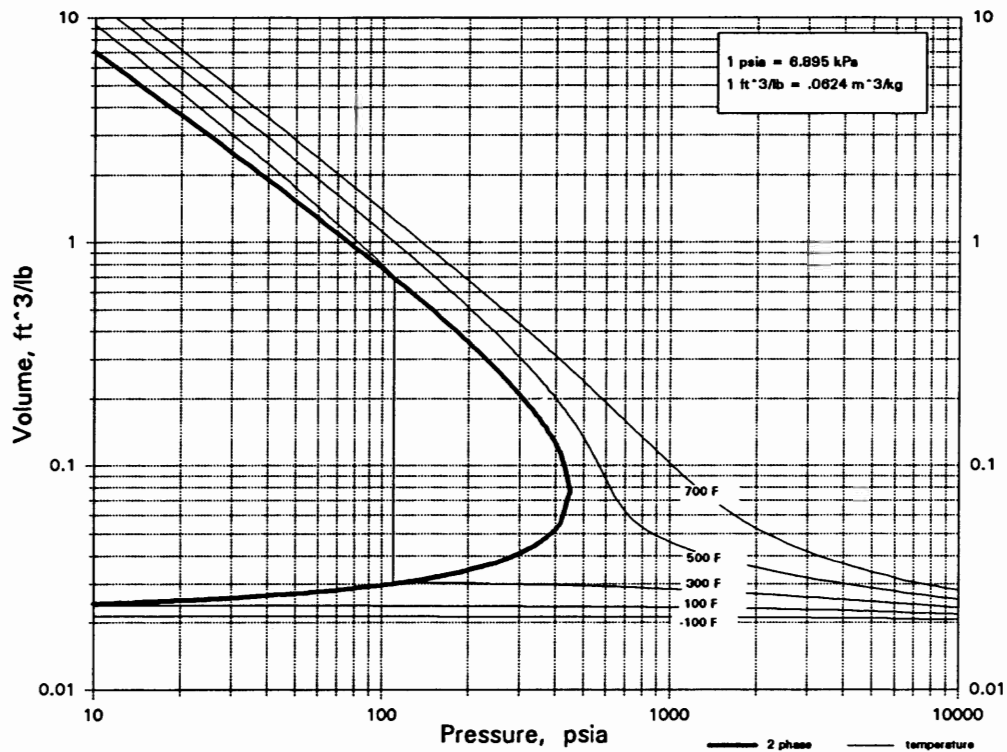
C6H14

2-METHYLPENTANE

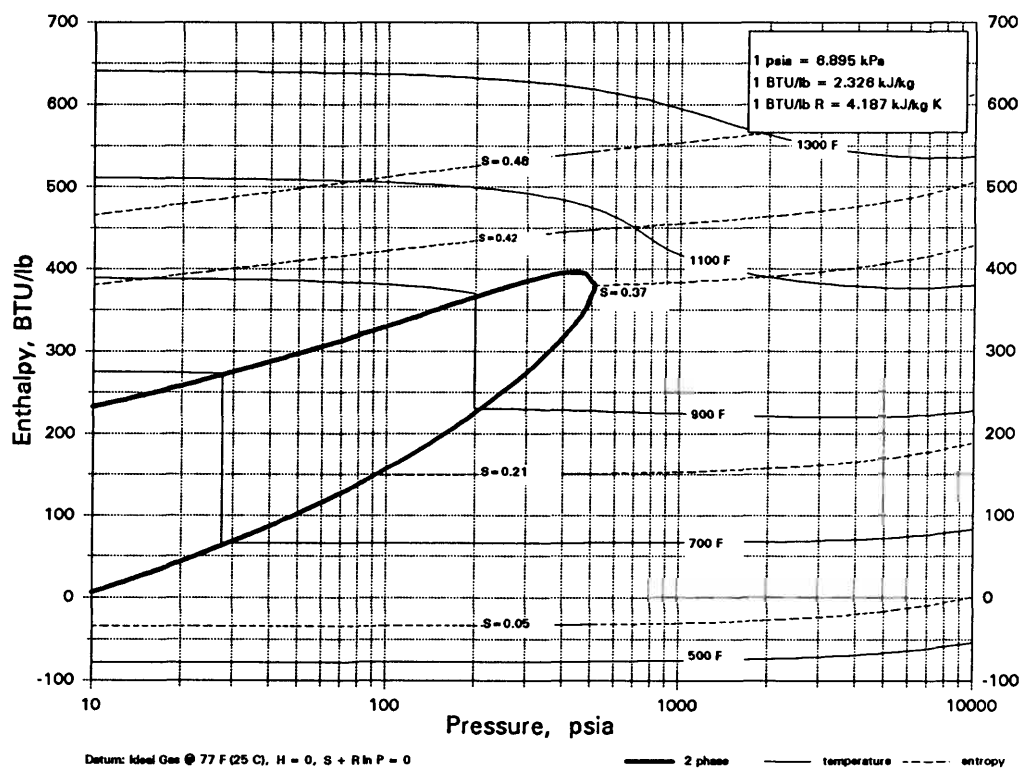
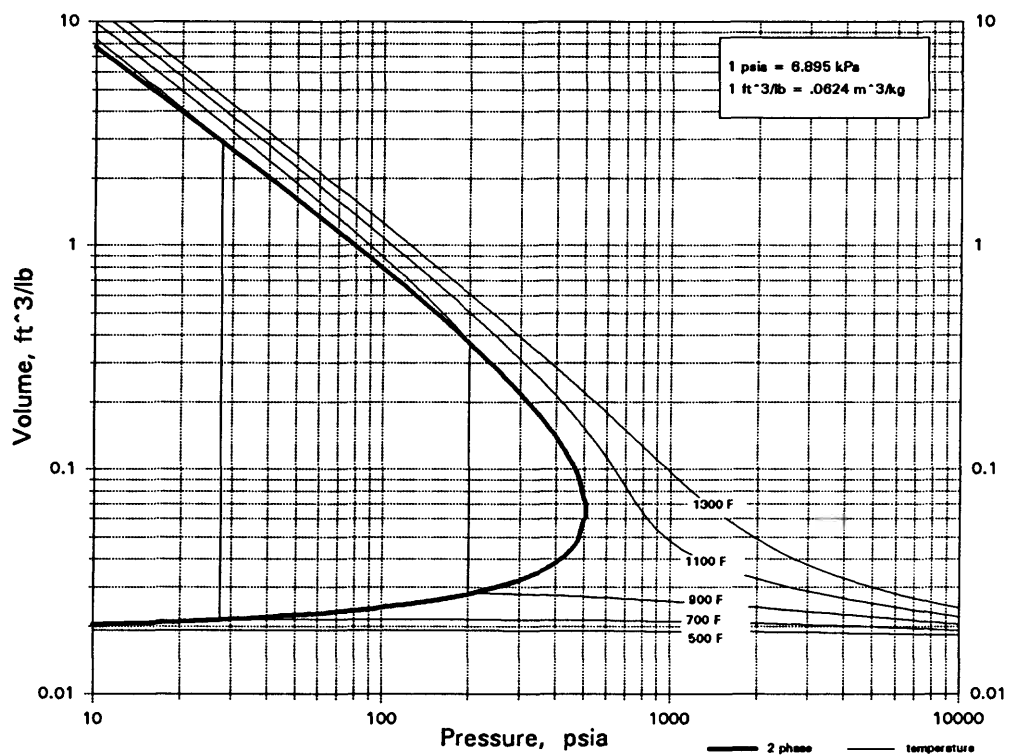


C6H14

3-METHYLPENTANE

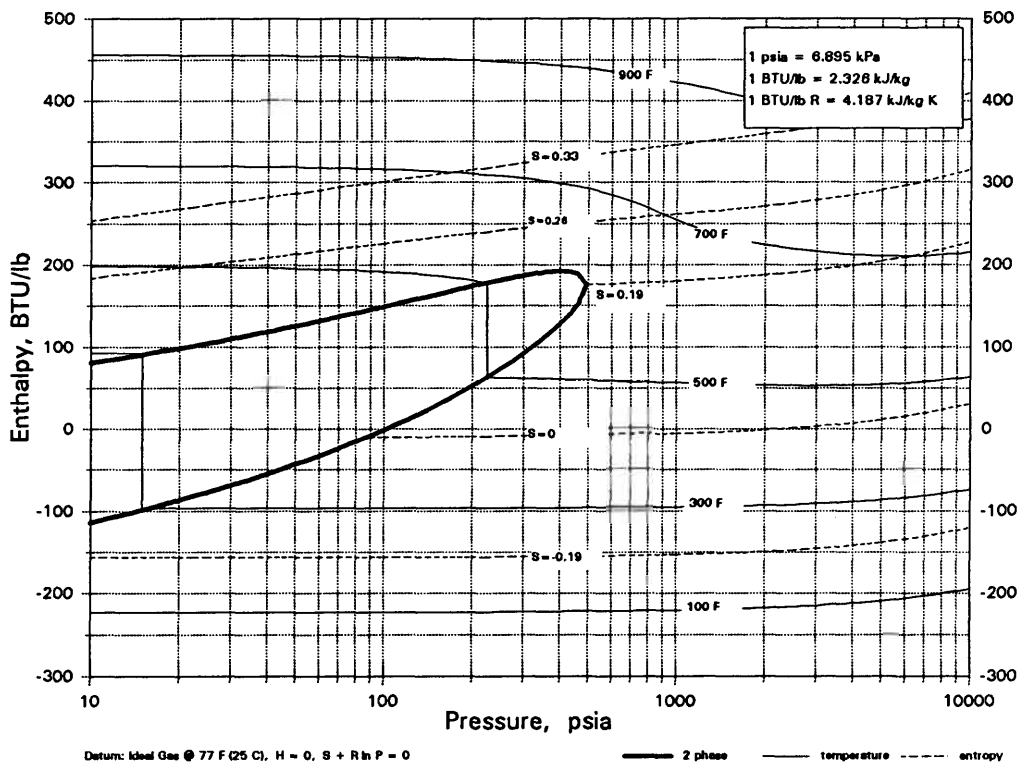
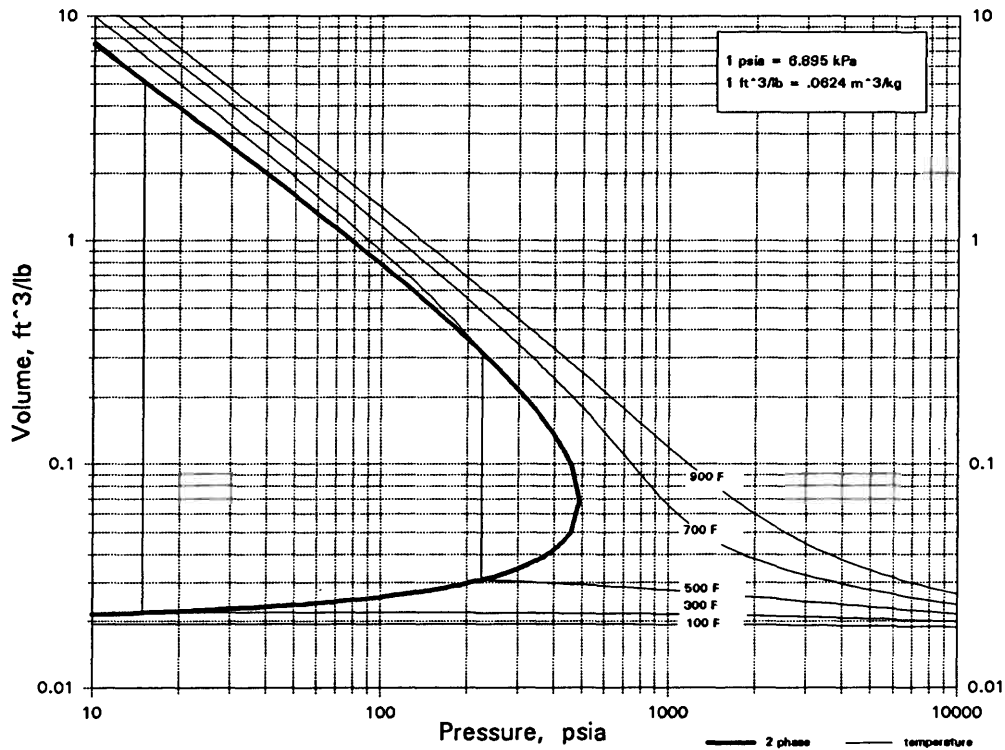


C6H14N2O2 LYSINE



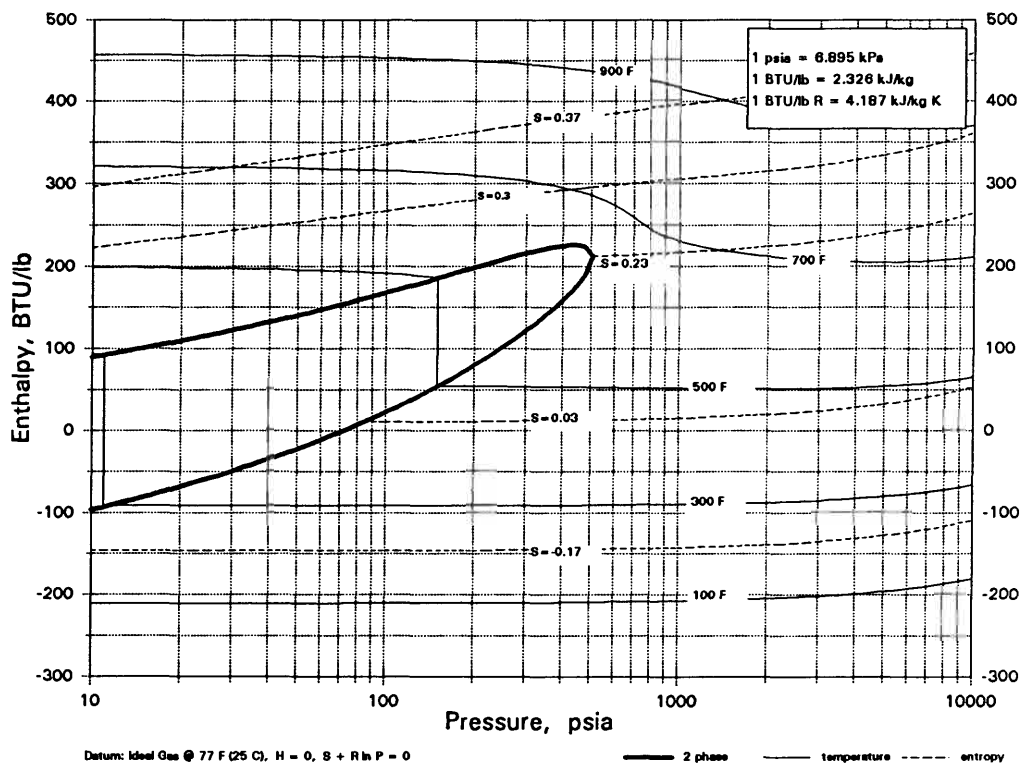
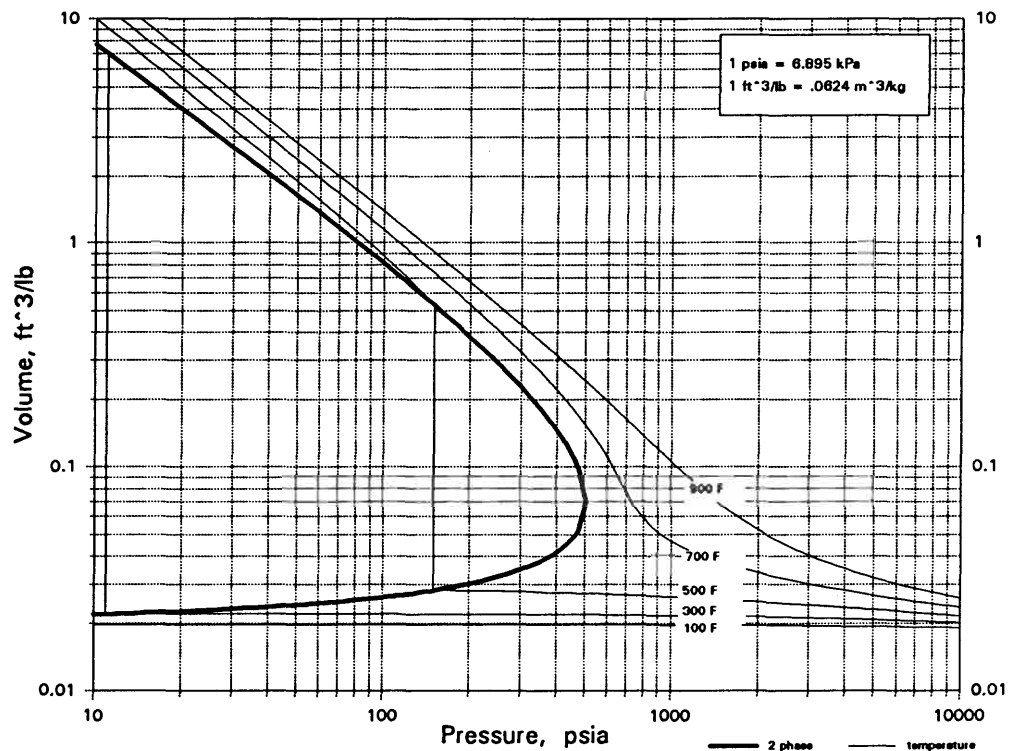
C6H14O

2-ETHYL-1-BUTANOL



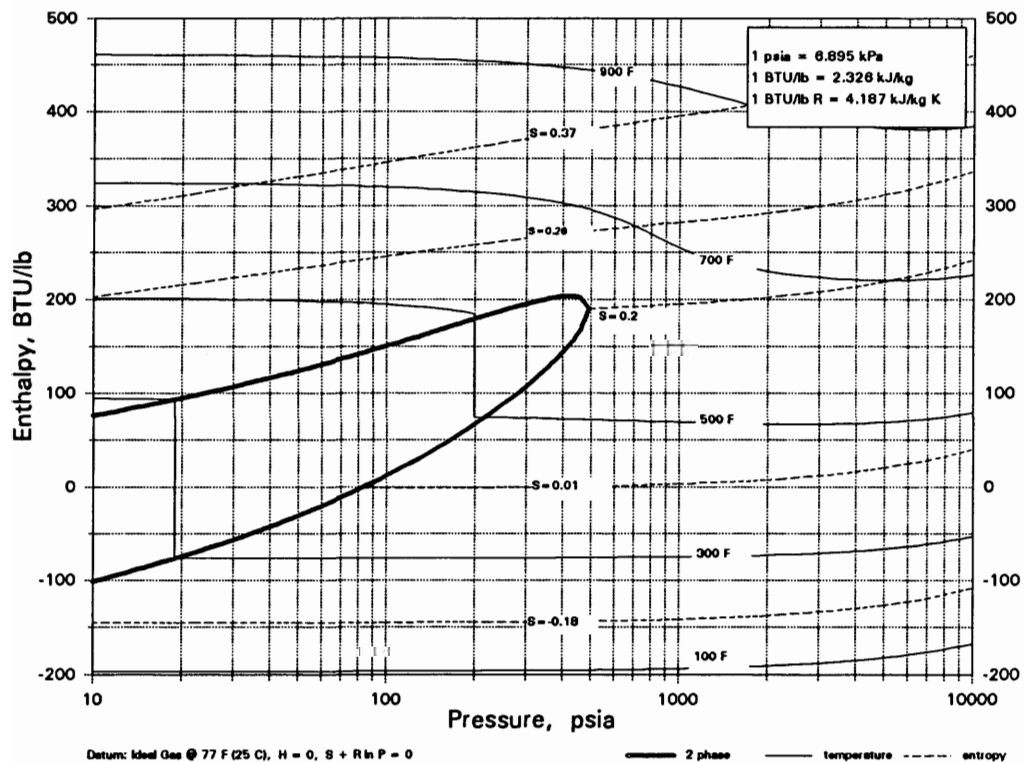
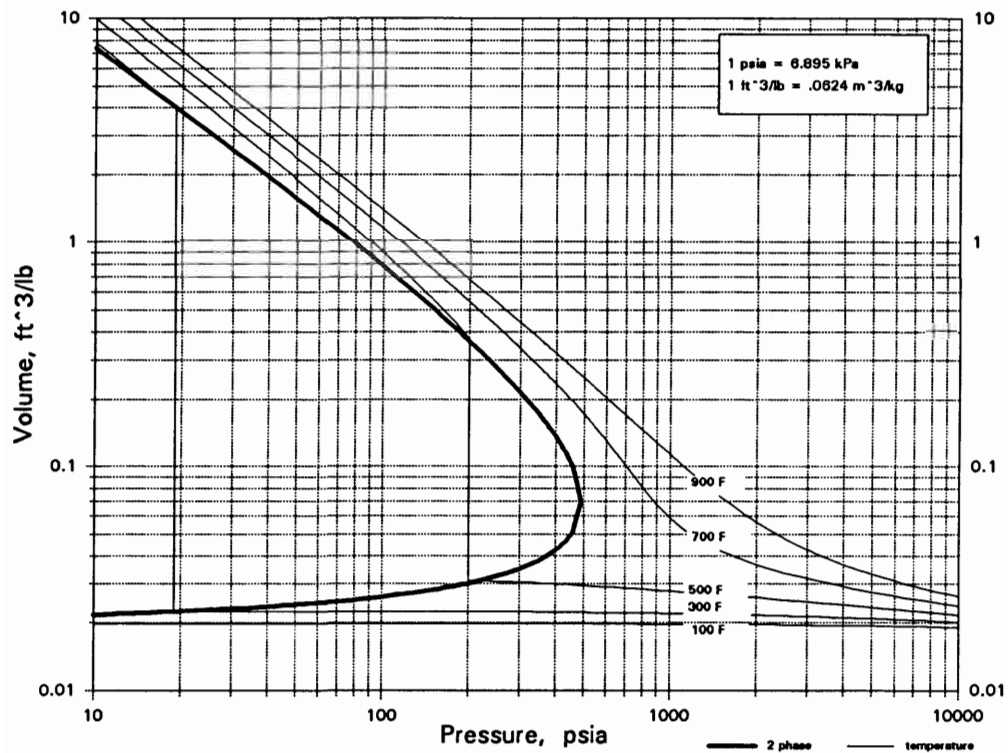
C6H14O

1-HEXANOL



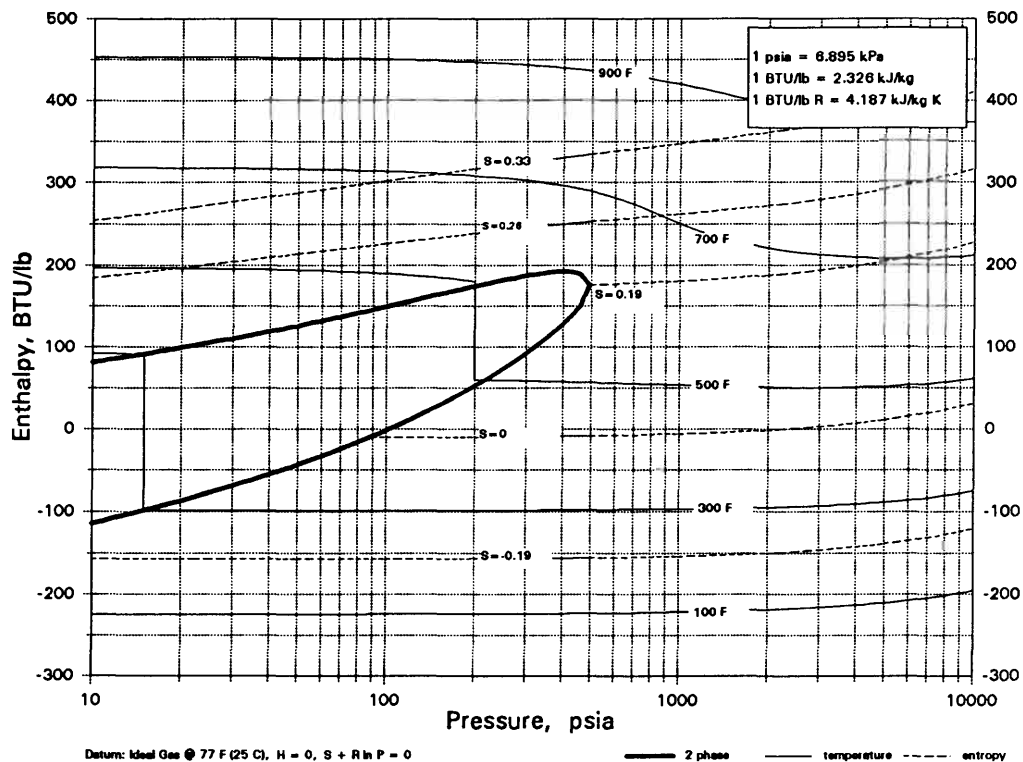
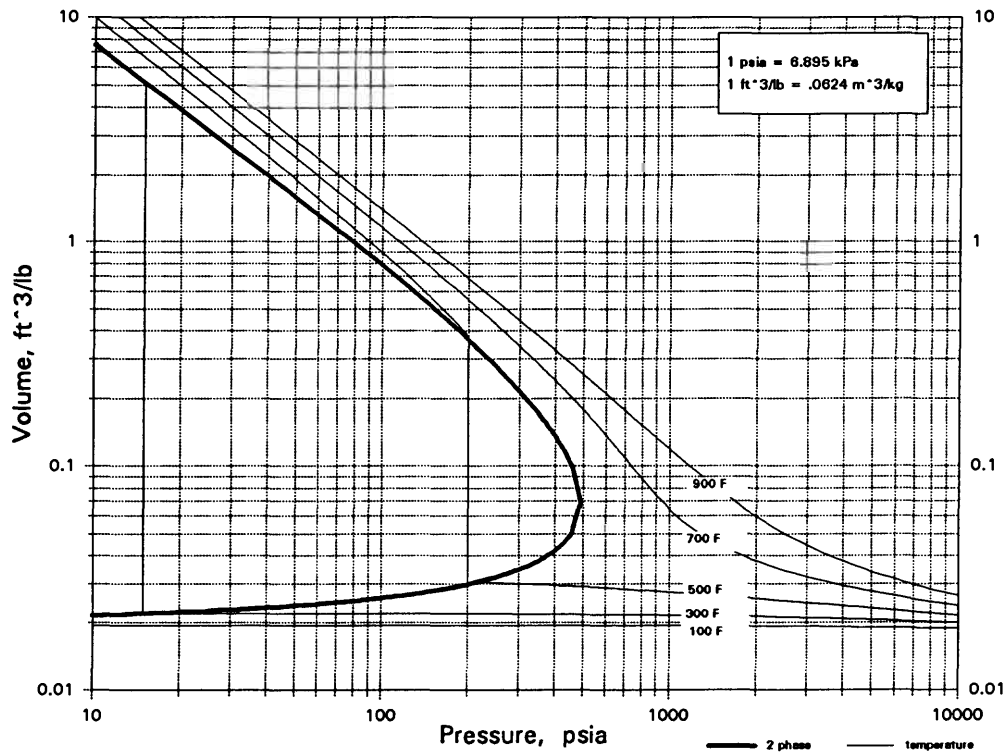
C6H14O

2-HEXANOL



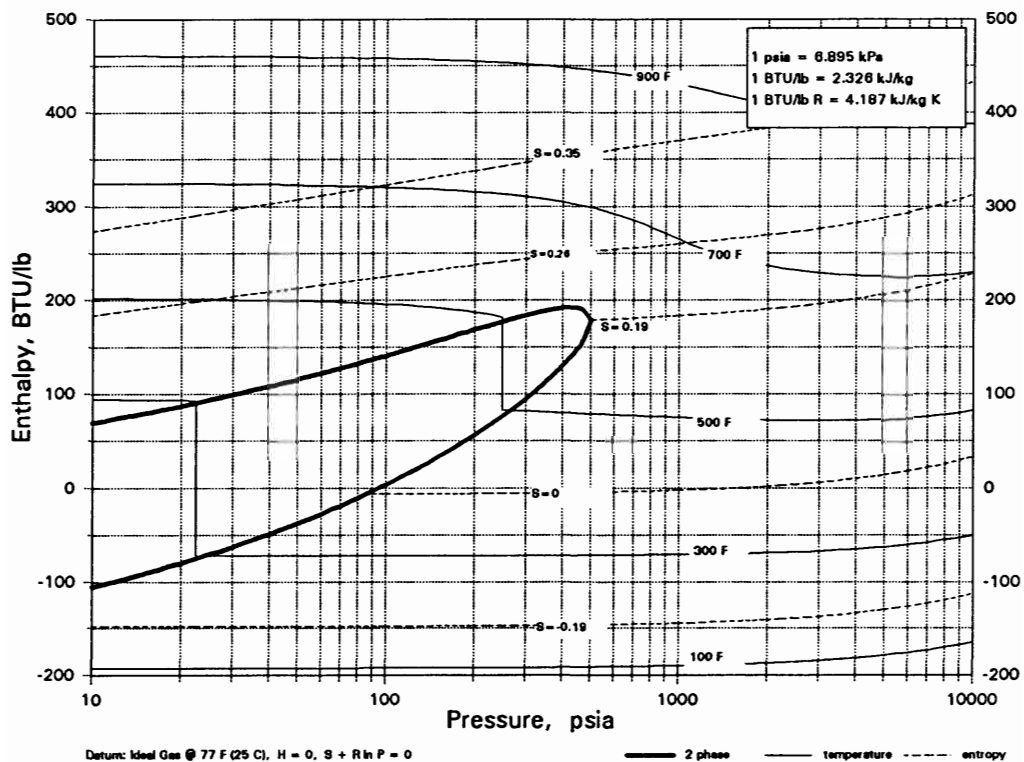
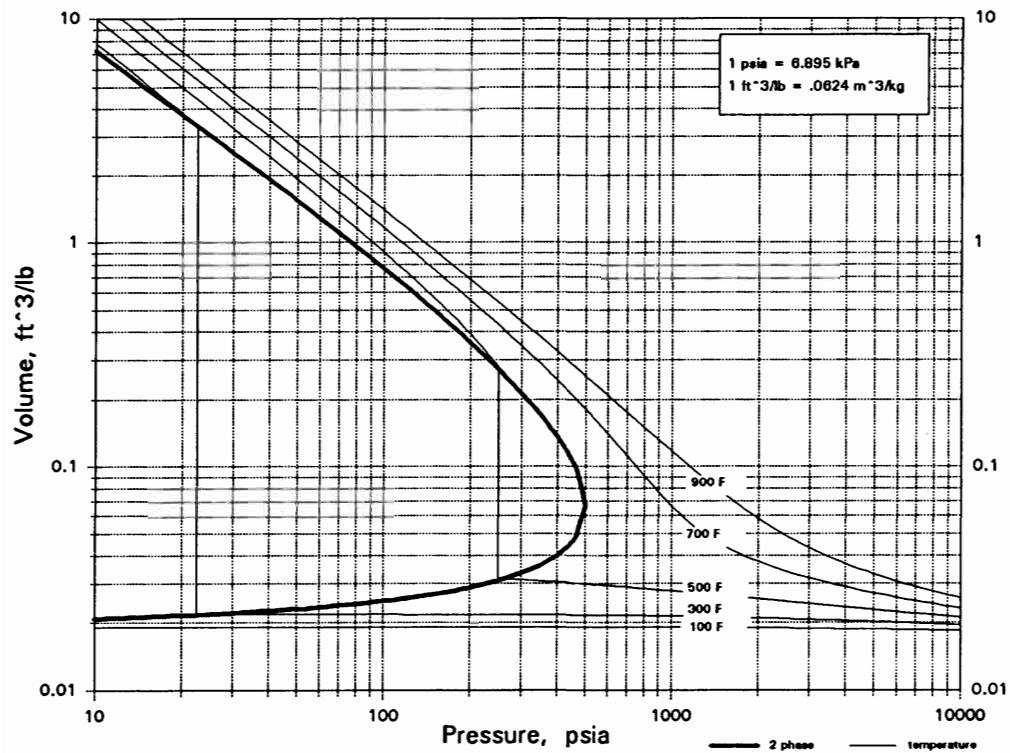
C6H14O

2-METHYL-1-PENTANOL



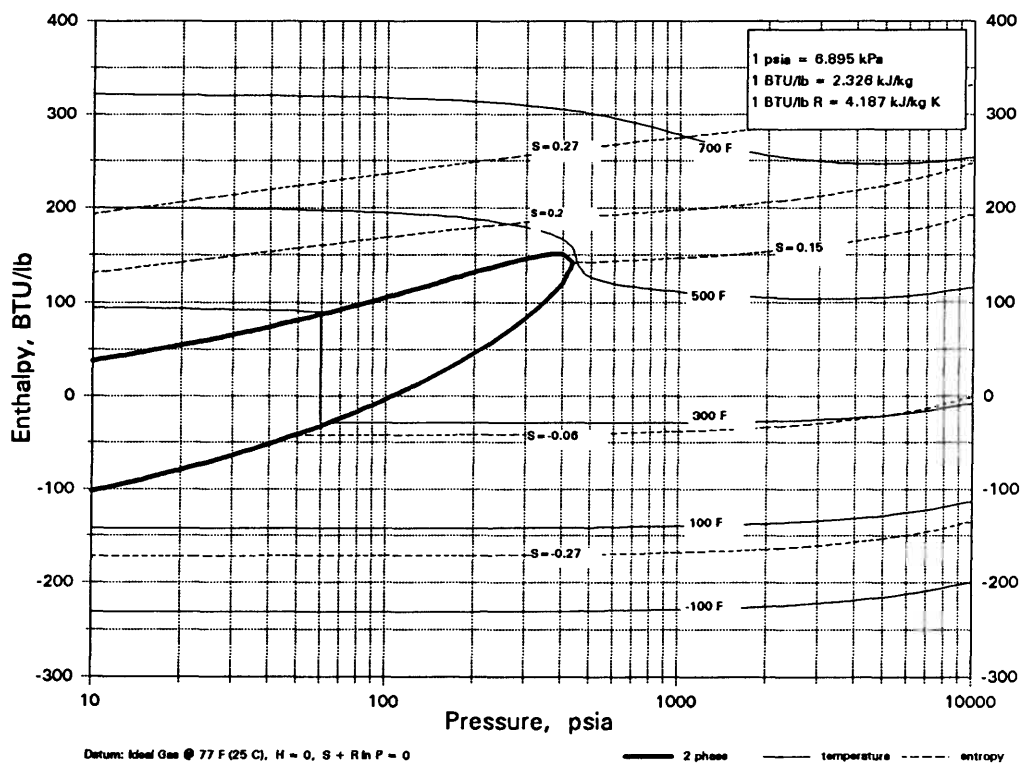
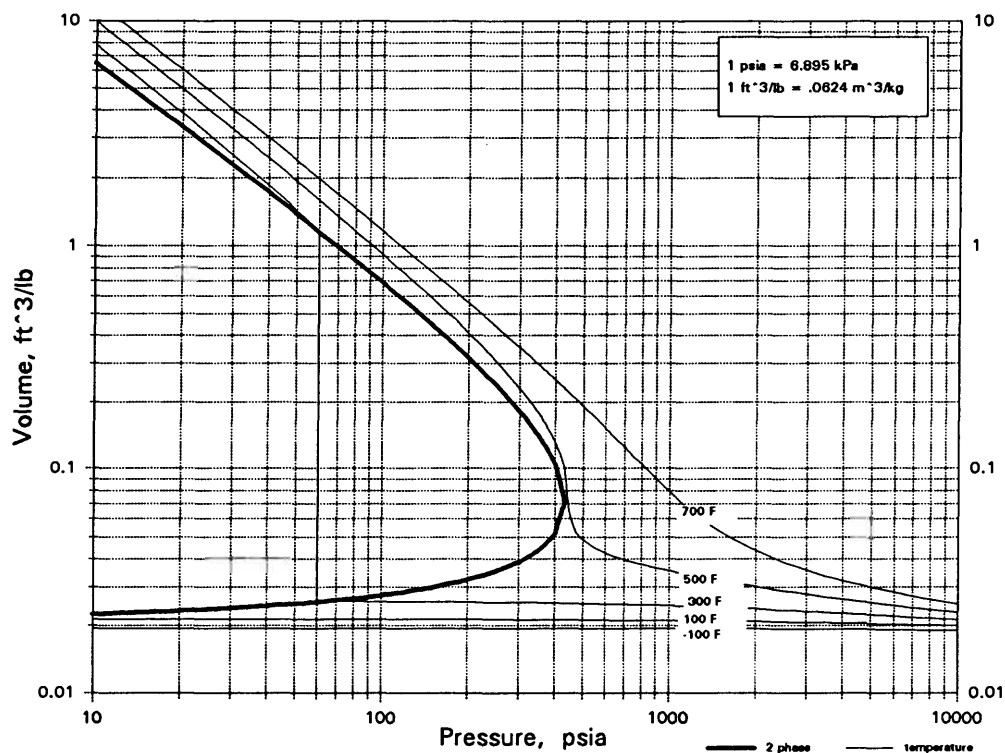
C6H14O

4-METHYL-2-PENTANOL



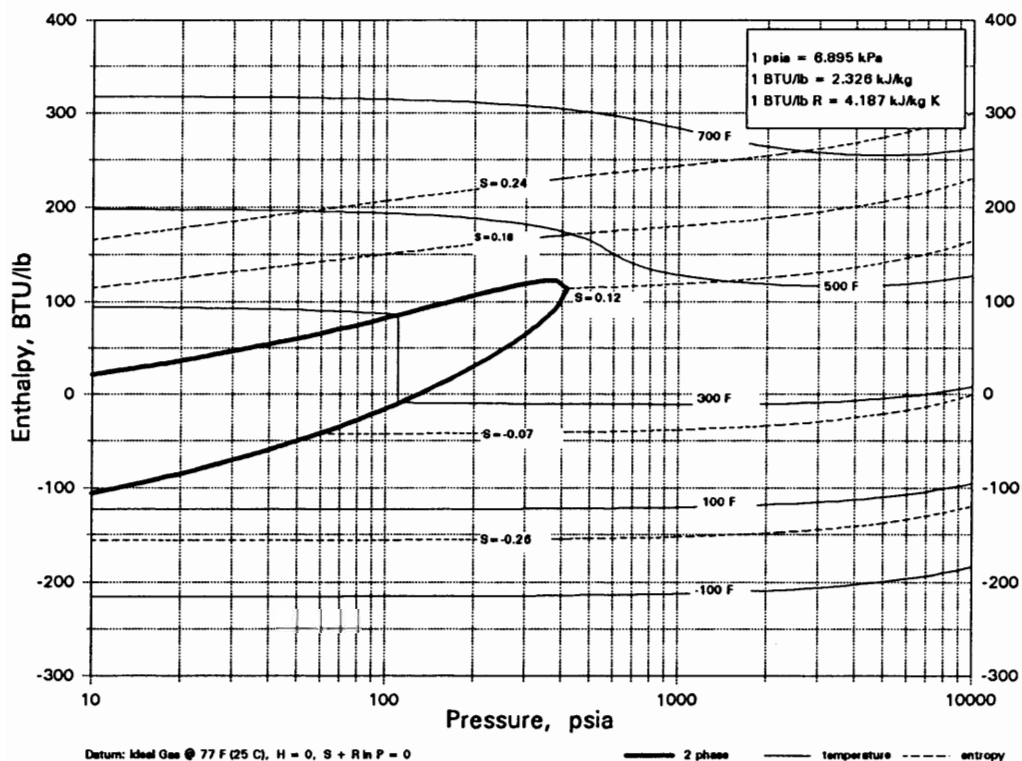
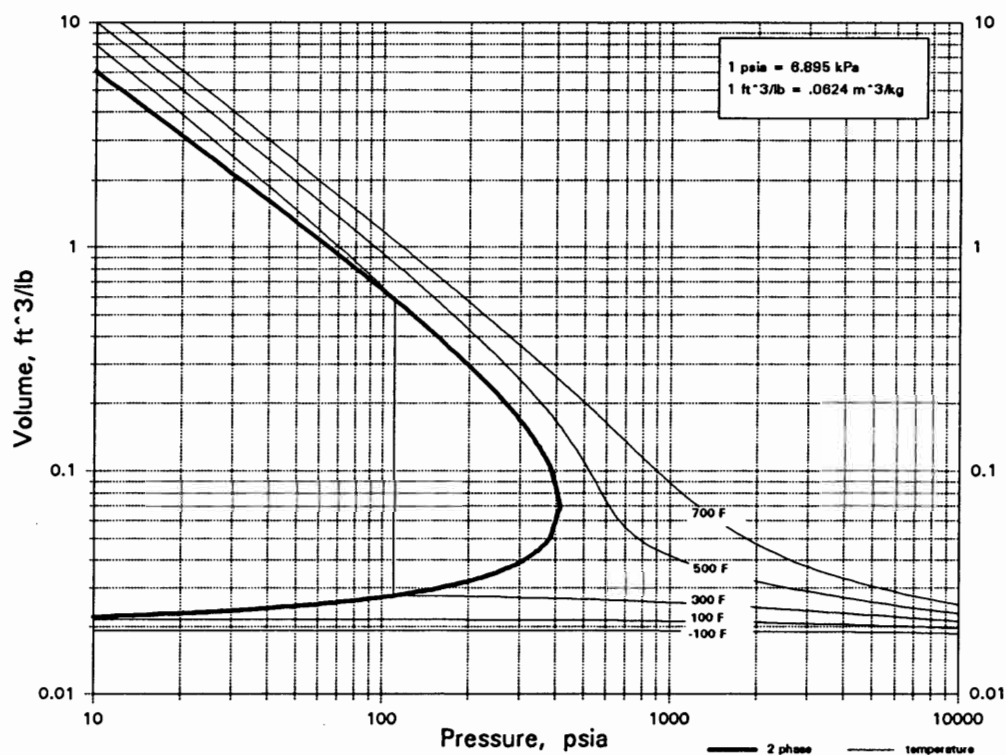
C6H14O

n-BUTYL ETHYL ETHER



C6H14O

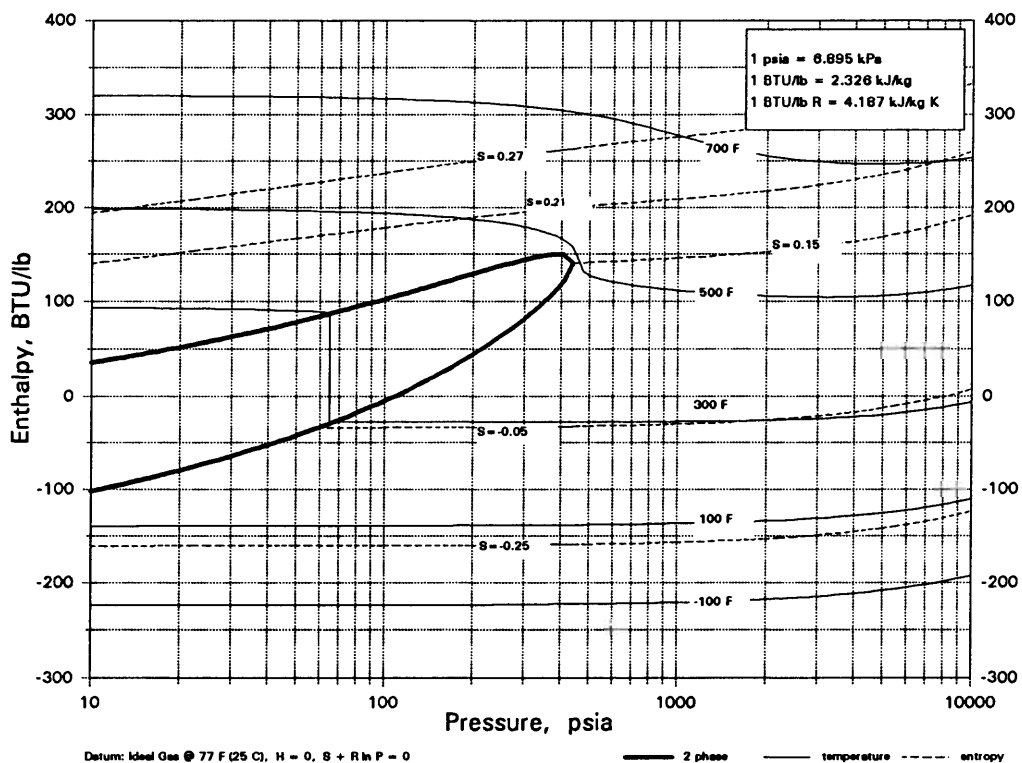
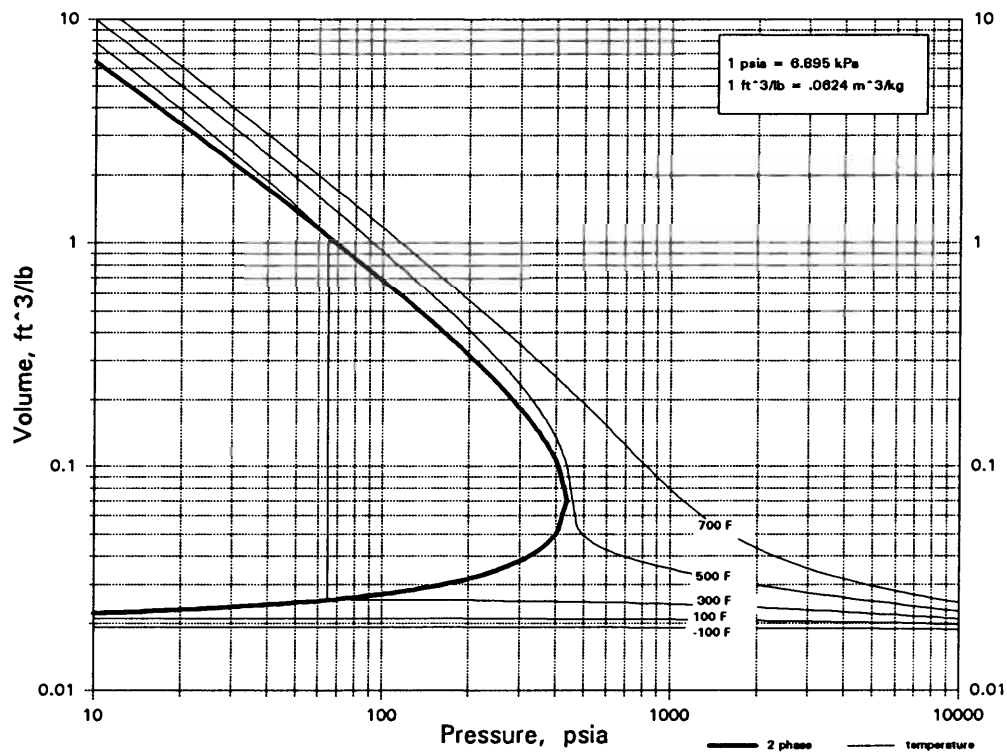
DIISOPROPYL ETHER



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

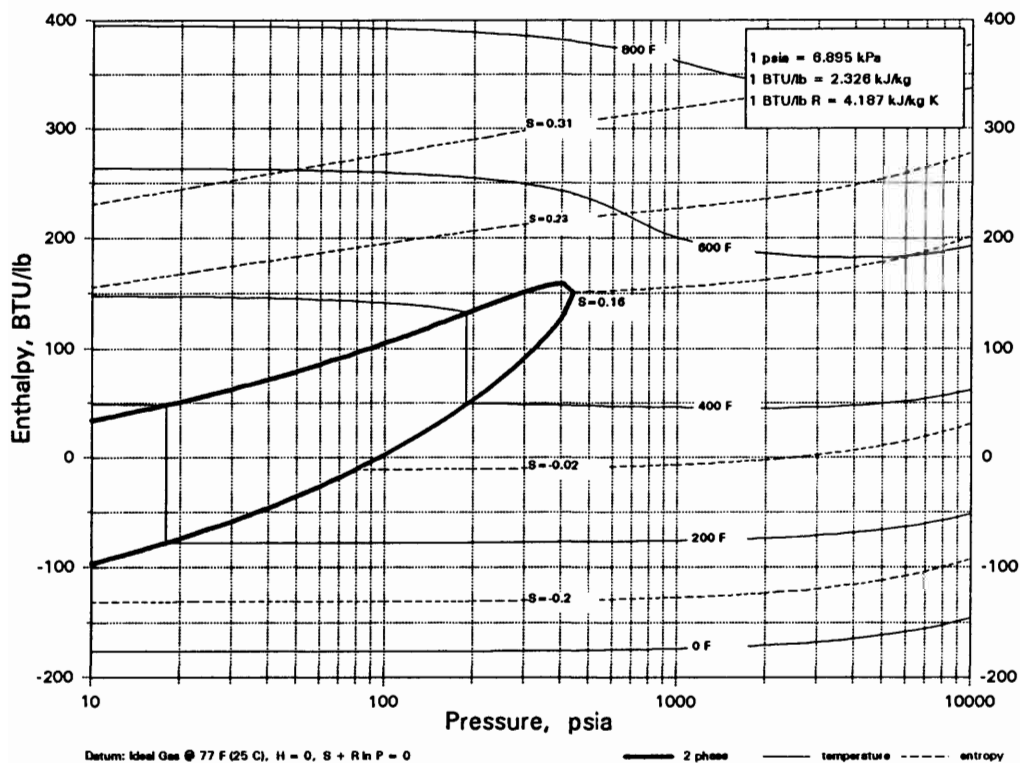
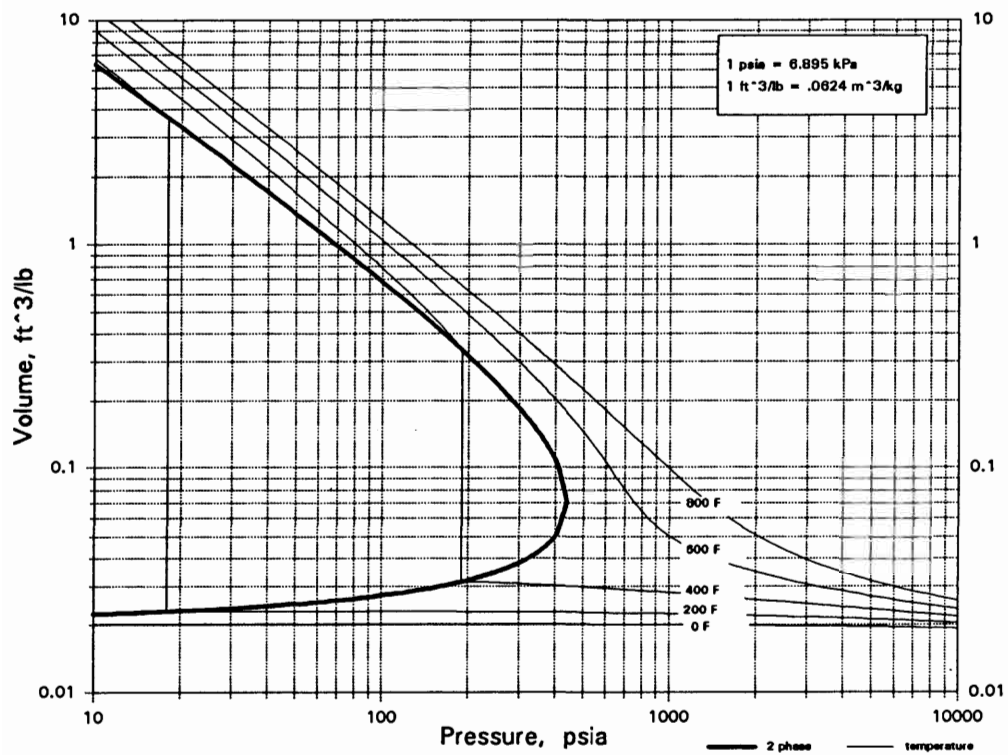
C6H14O

DI-n-PROPYL ETHER



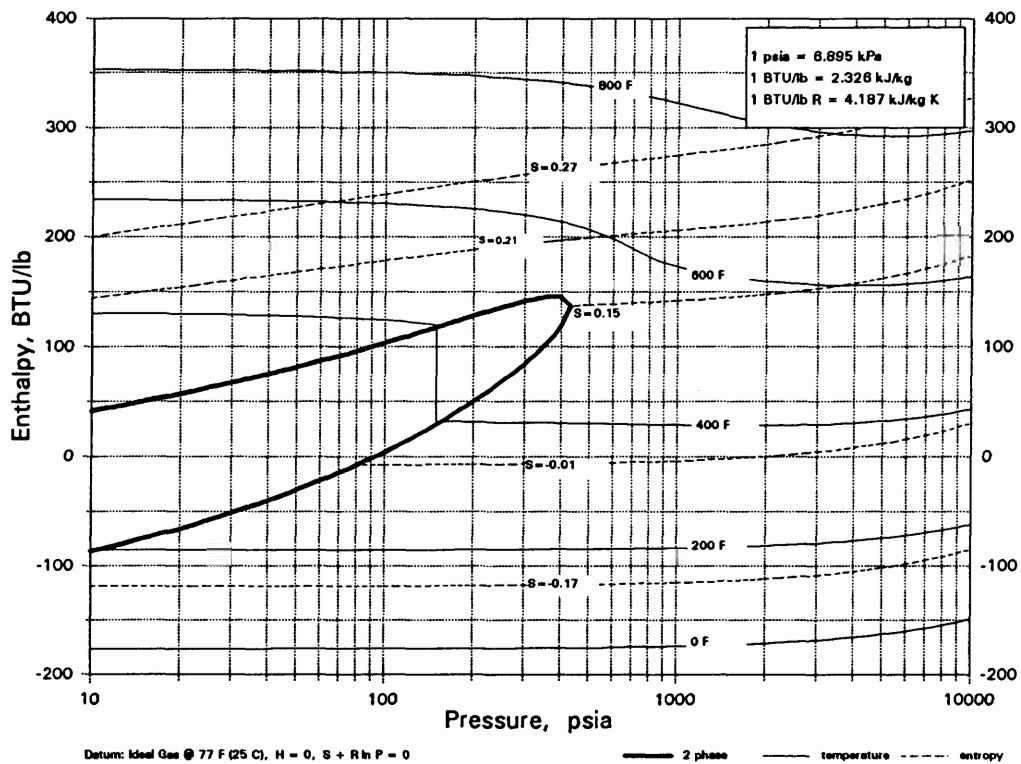
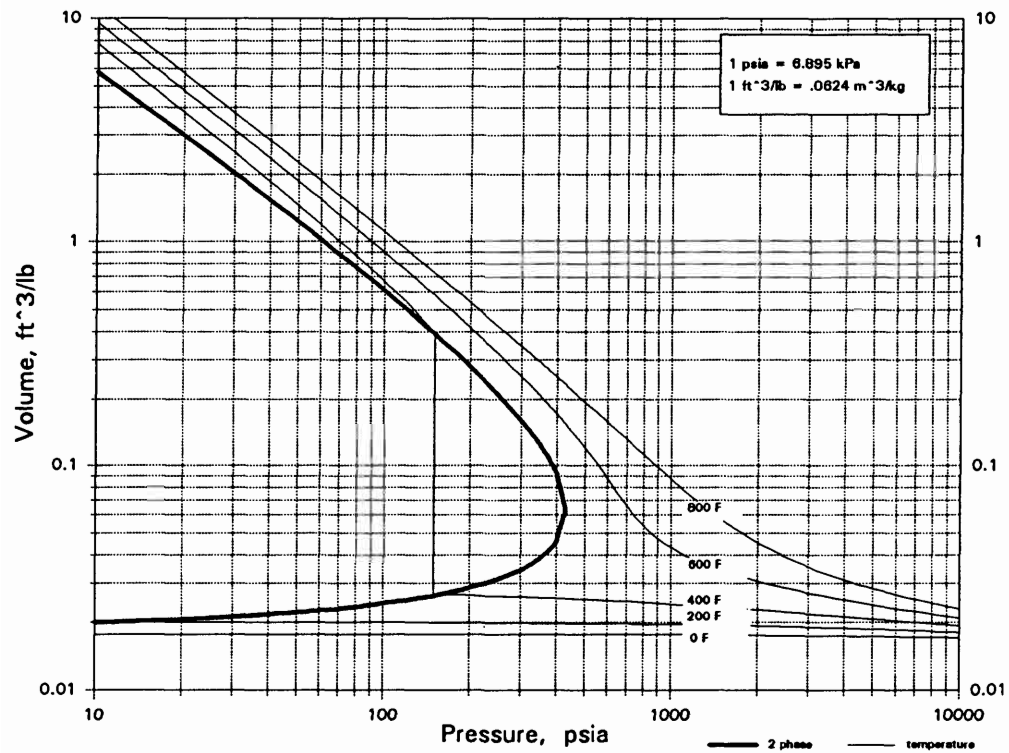
C6H14O

METHYL tert-PENTYL ETHER



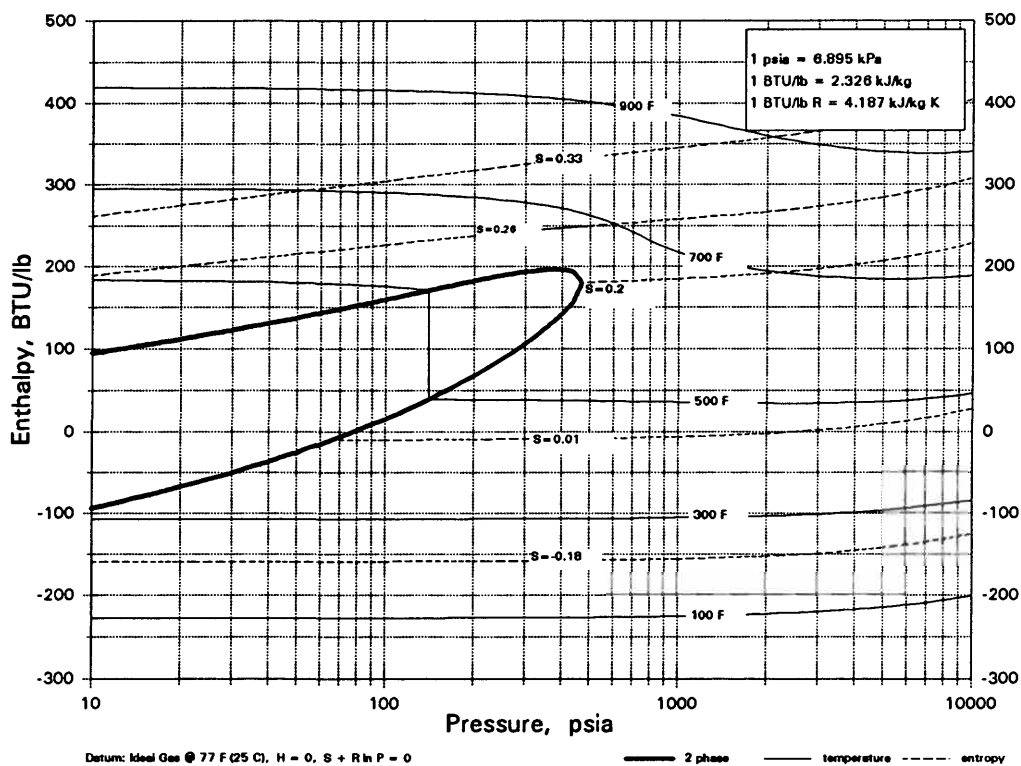
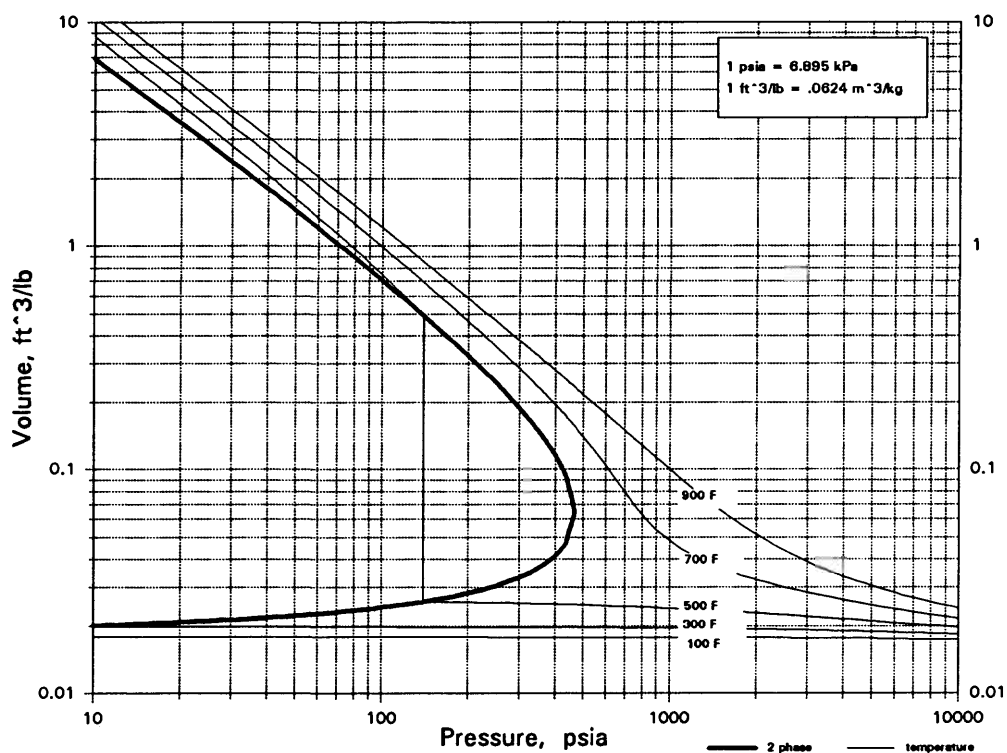
C6H14O2

ACETAL



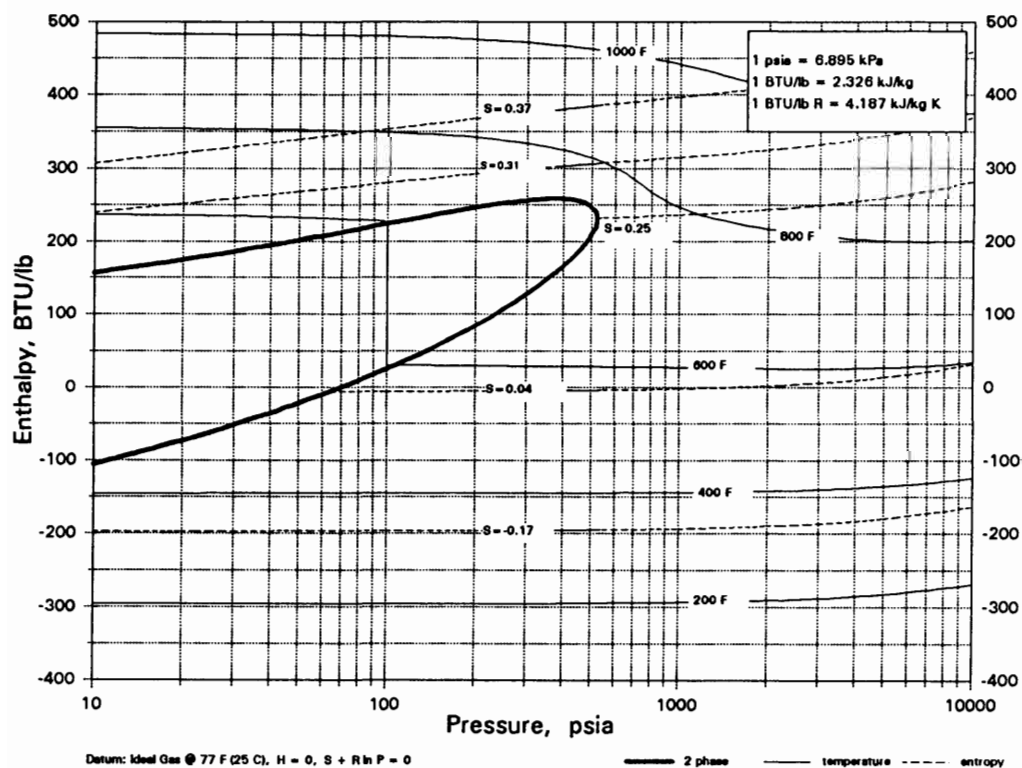
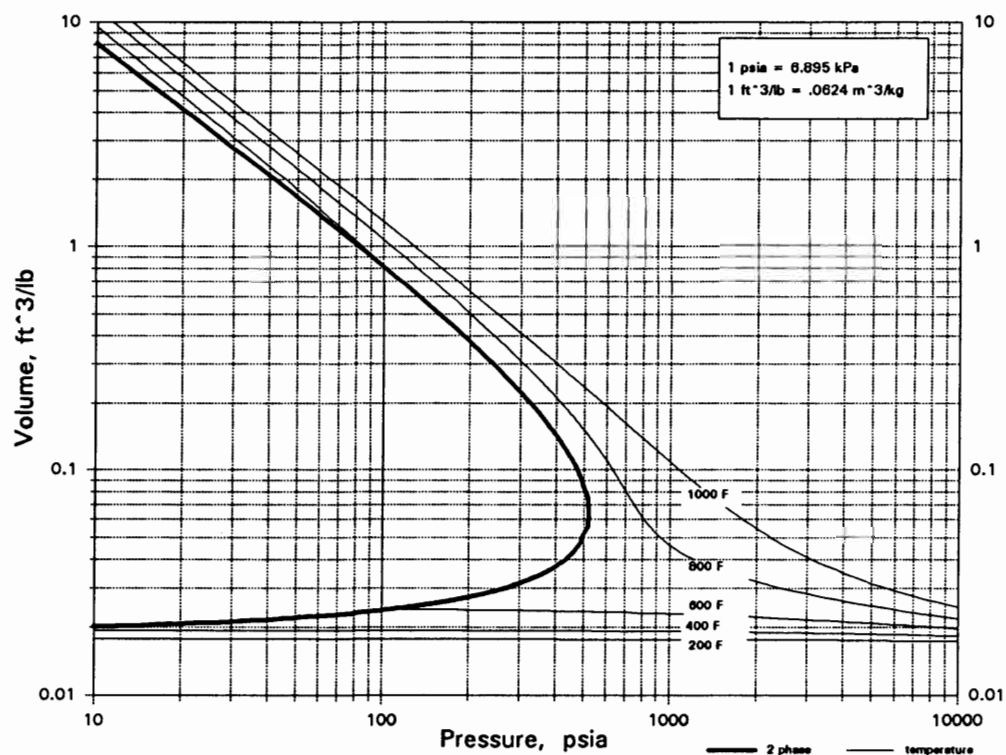
C6H14O2

2-BUTOXYETHANOL



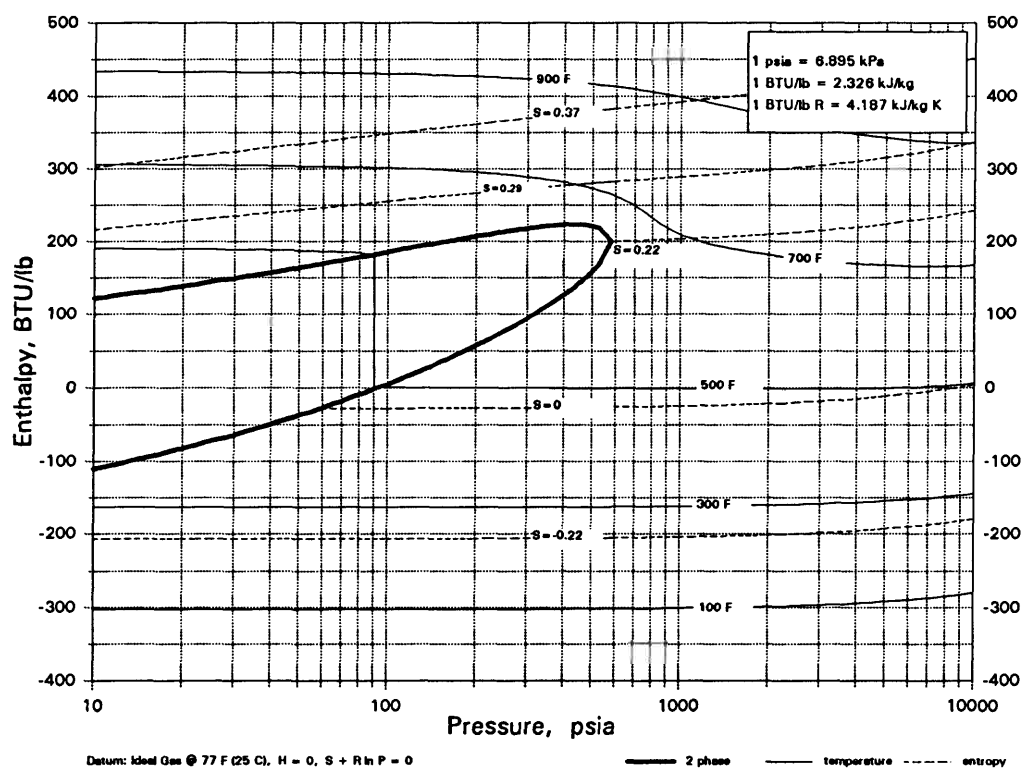
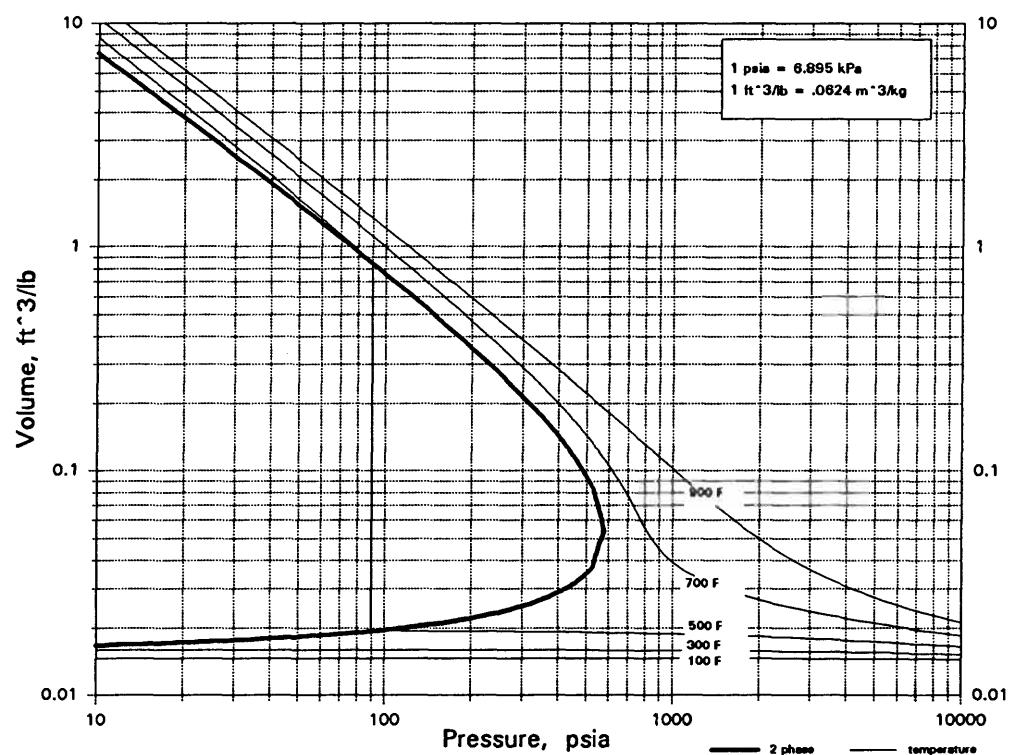
C6H14O2

1-6-HEXANEDIOL



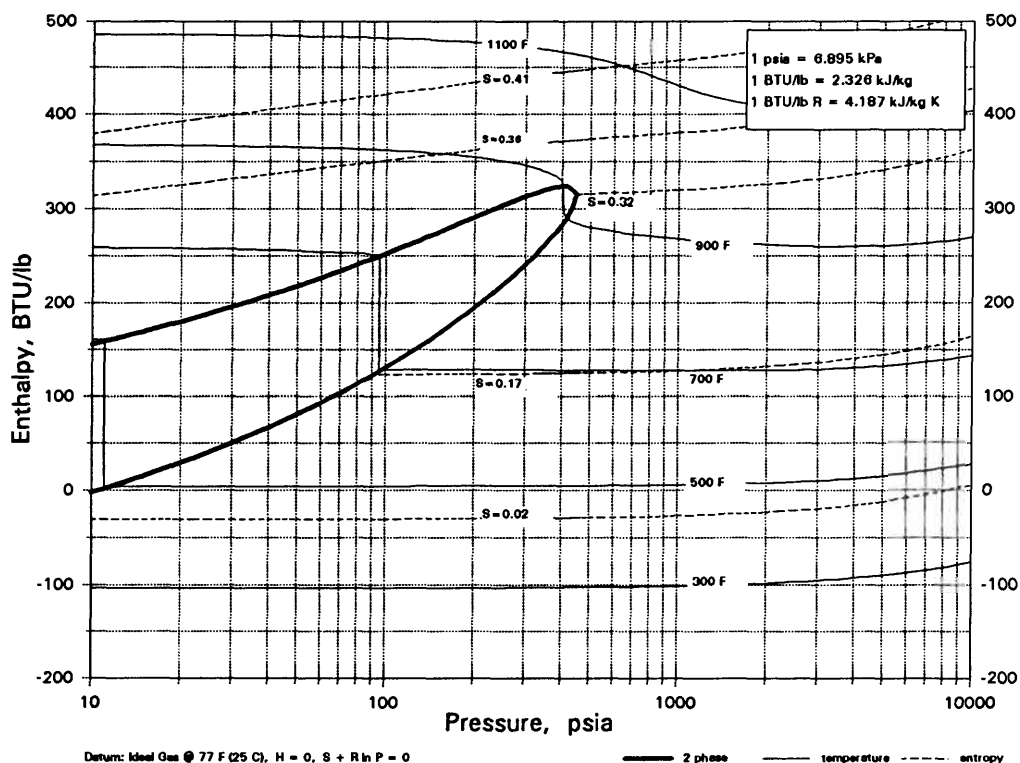
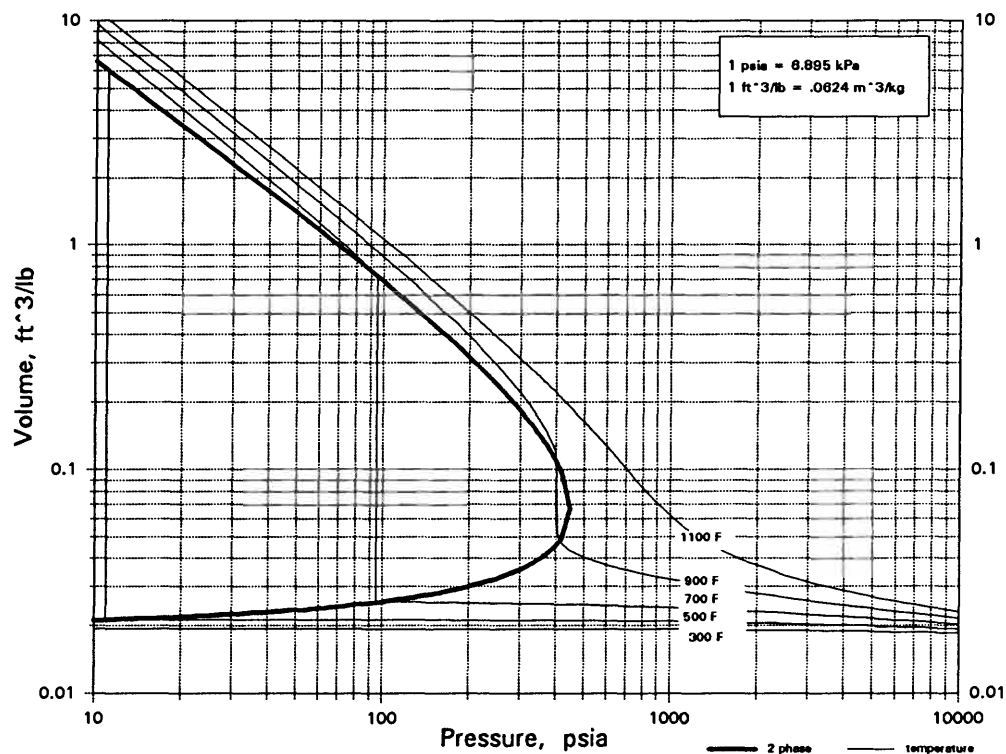
C6H14O2

HEXYLENE GLYCOL



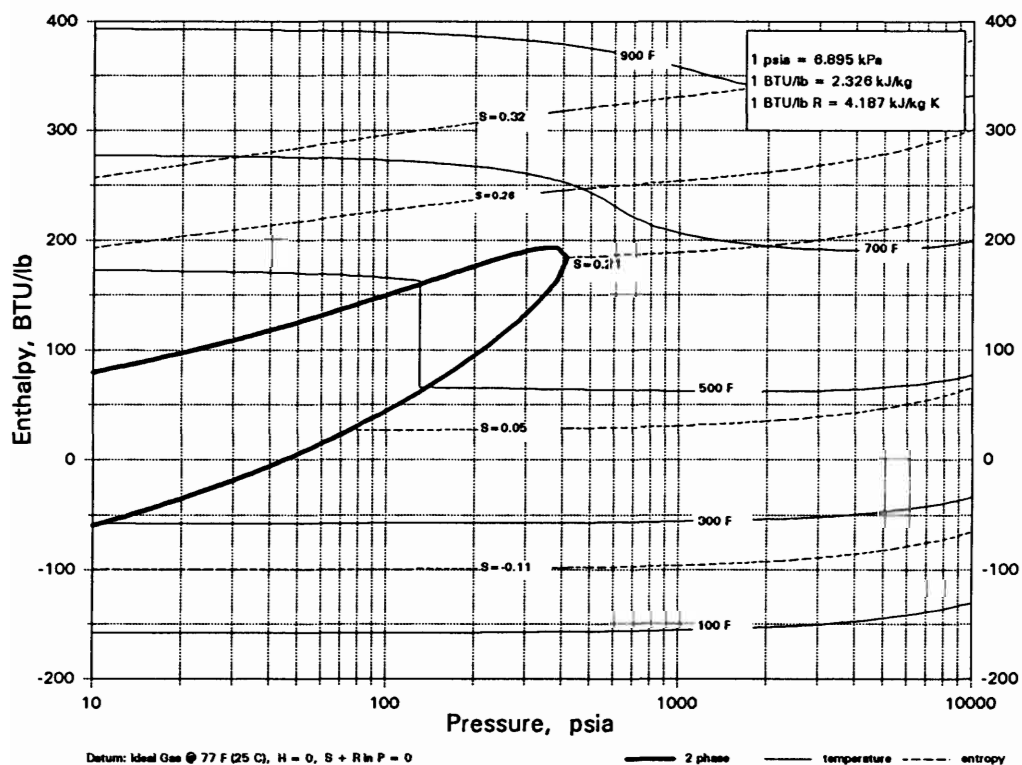
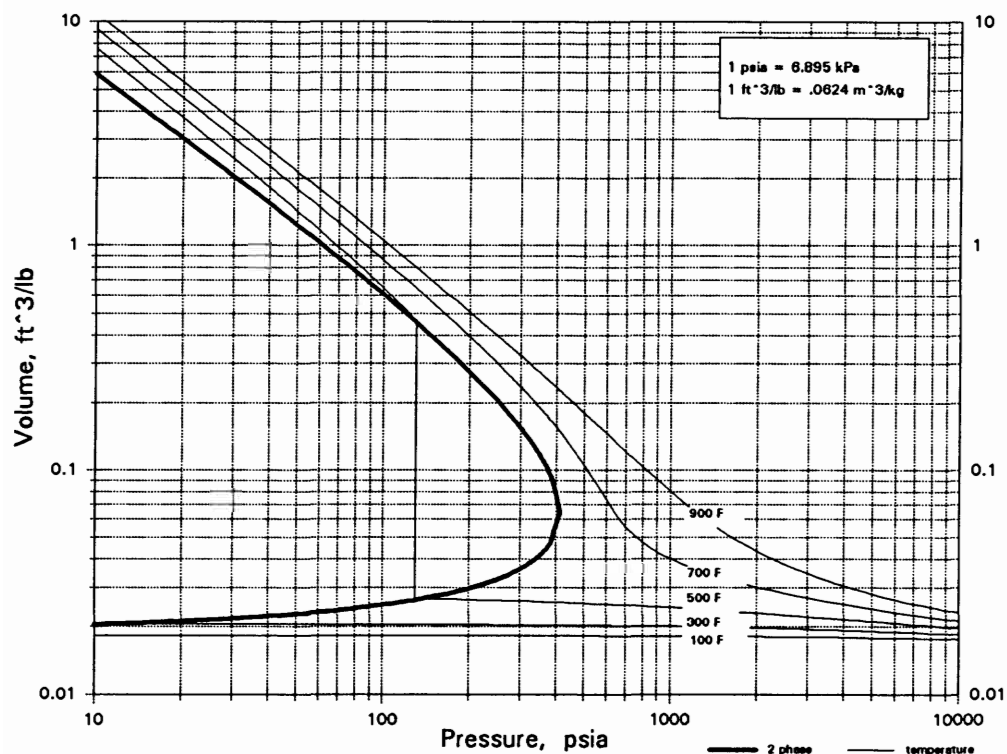
C6H14O2S

DI-n-PROPYL SULFONE

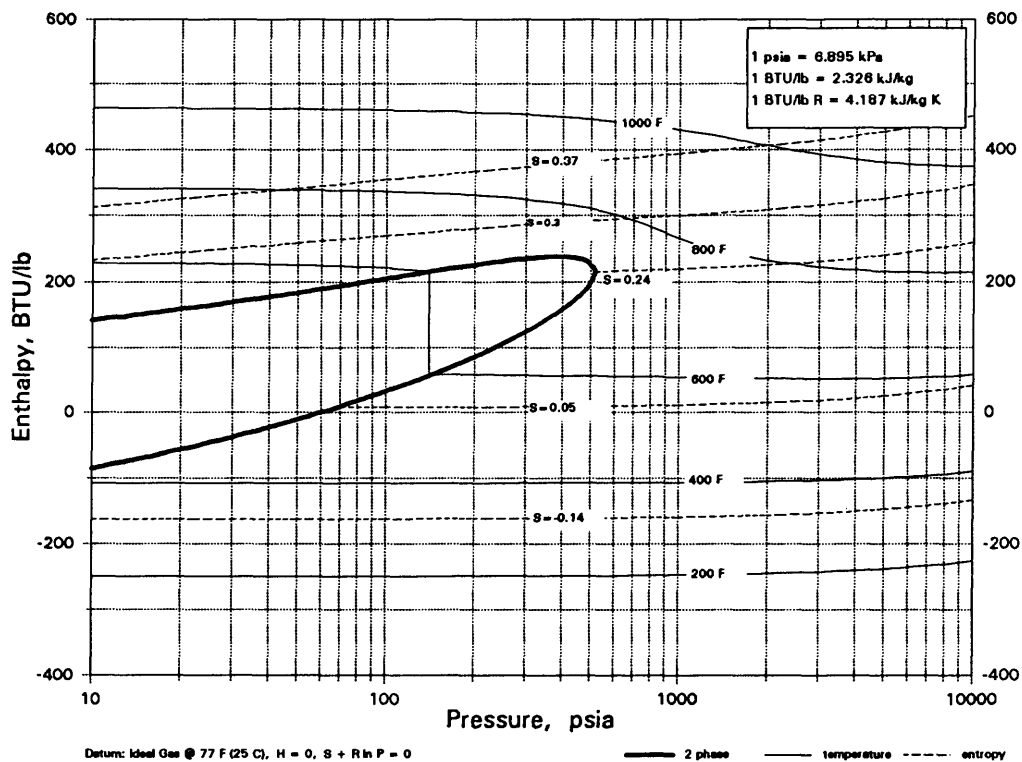
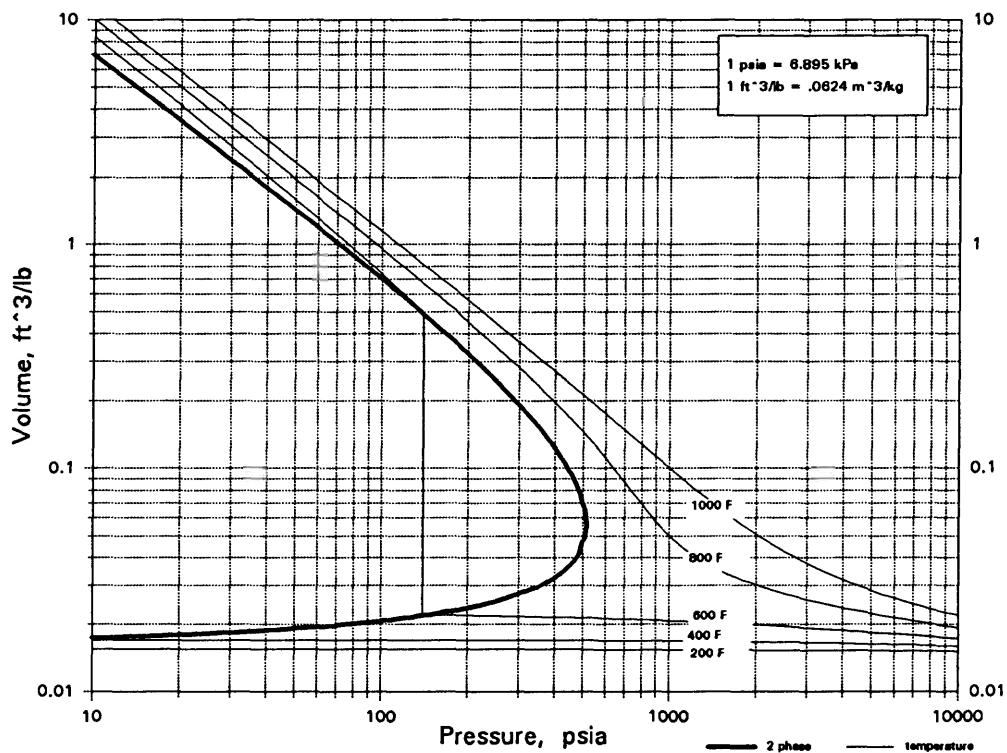


C6H14O3

DIETHYLENE GLYCOL DIMETHYL ETHER

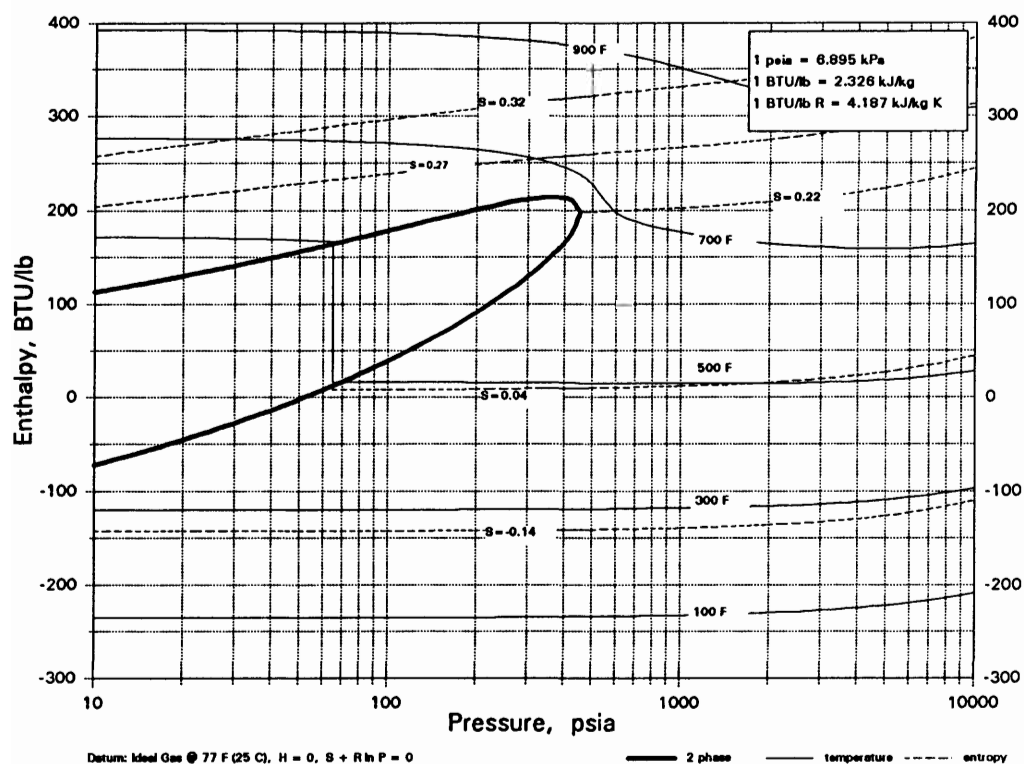
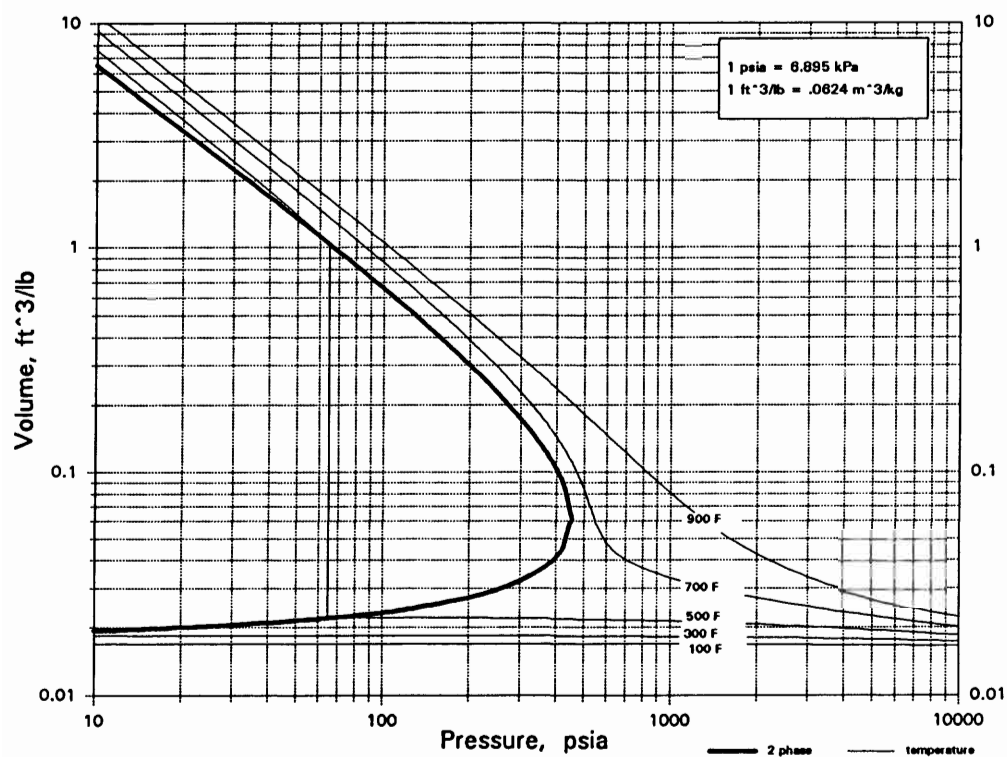


C6H14O3
DIPROPYLENE GLYCOL



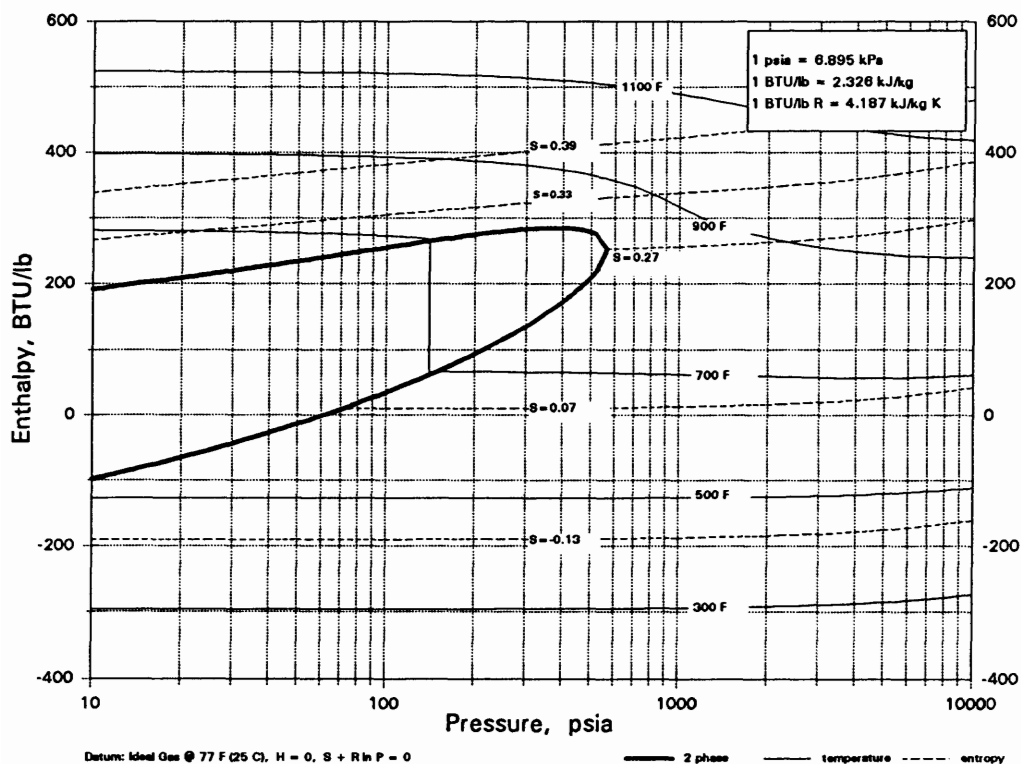
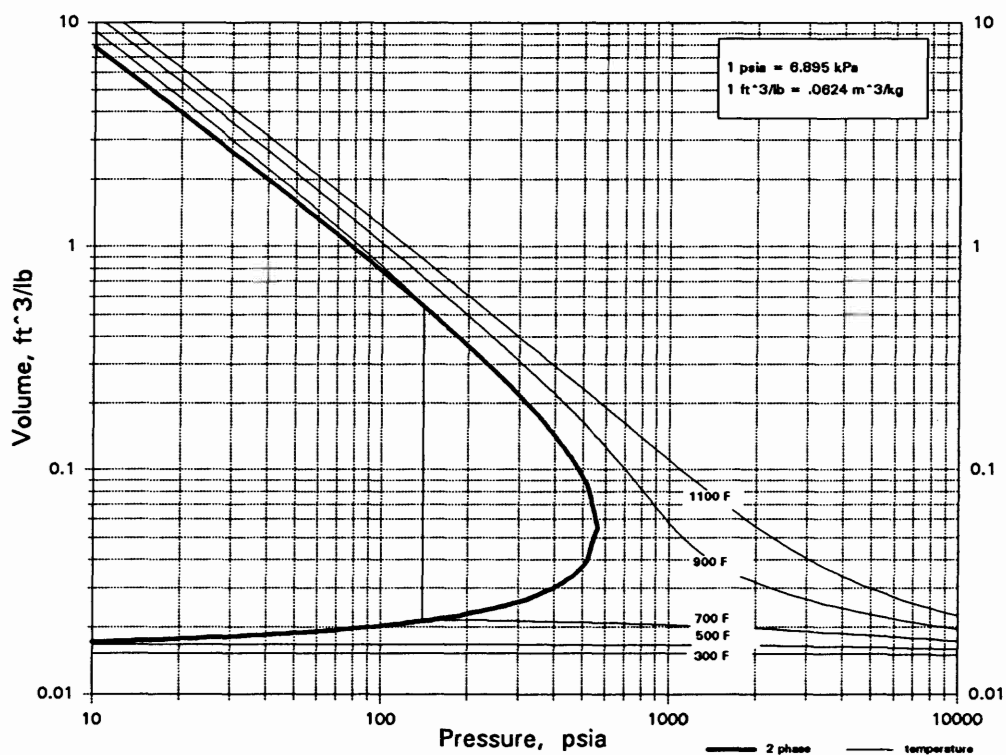
C6H14O3

2-(2-ETHOXYETHOXY)ETHANOL



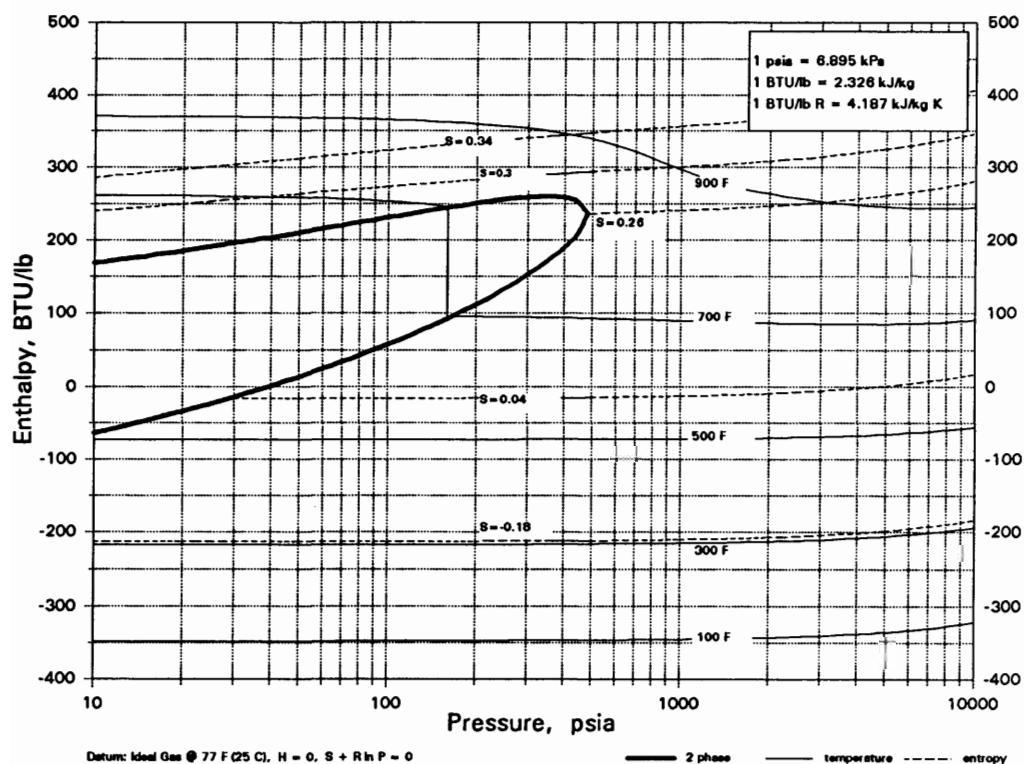
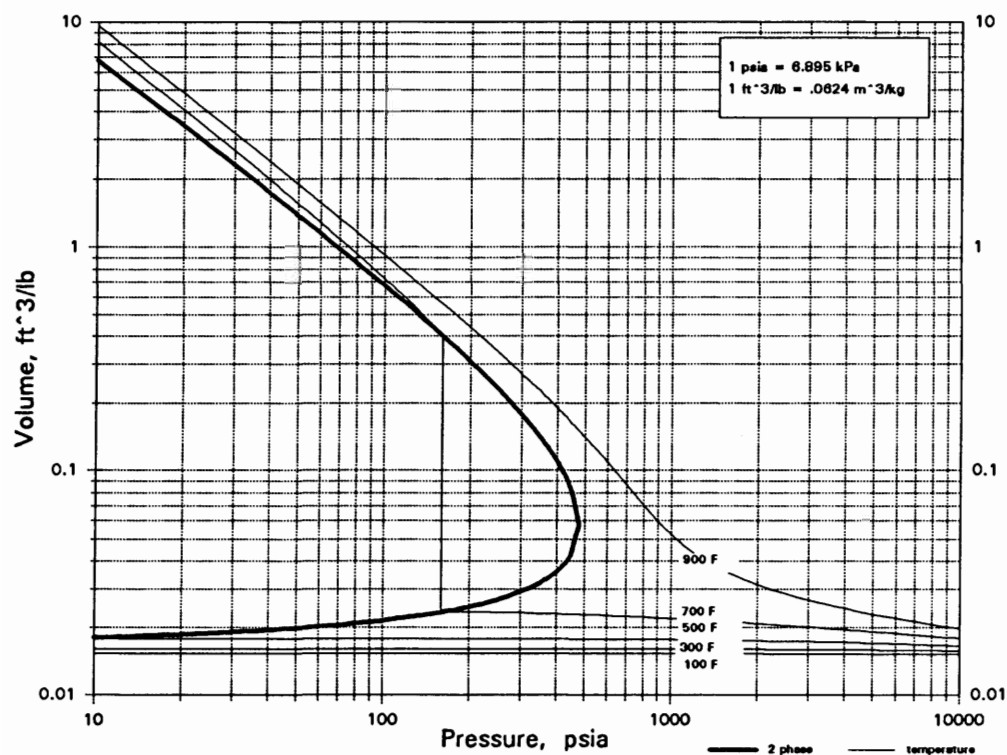
C6H14O3

TRIMETHYLOLPROPANE



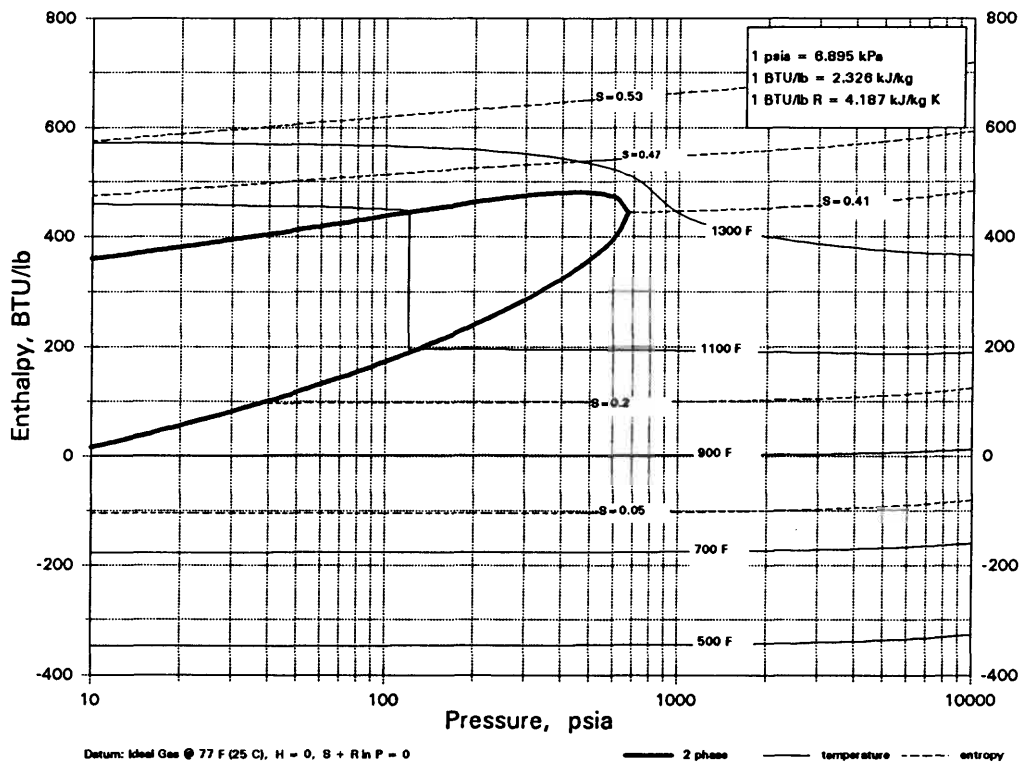
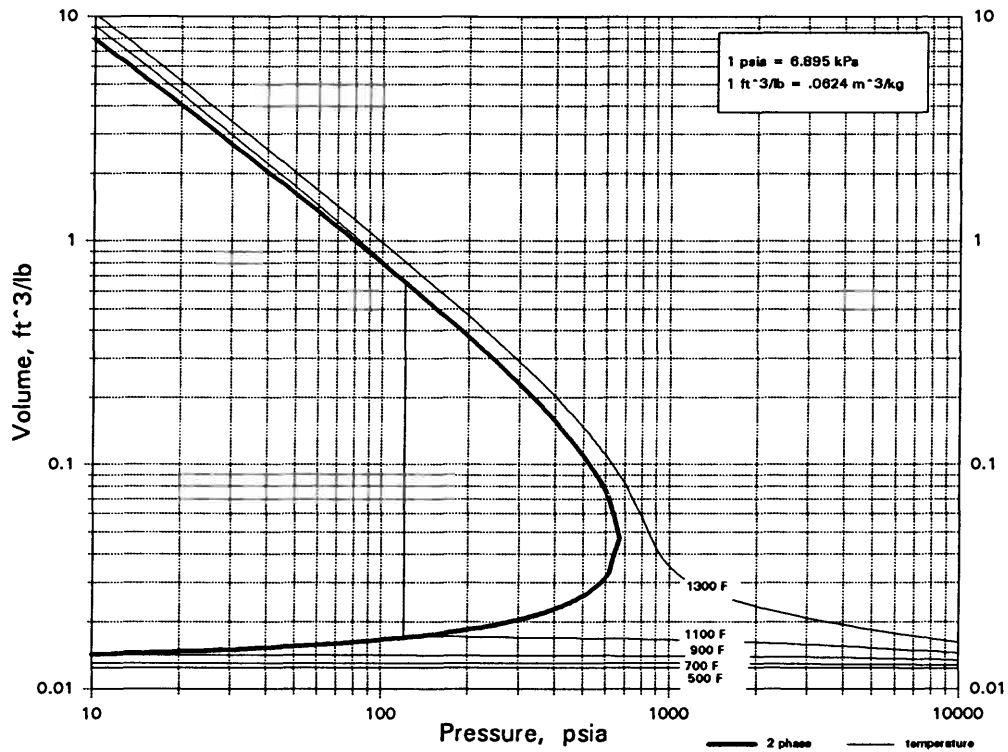
C6H14O4

TRIETHYLENE GLYCOL



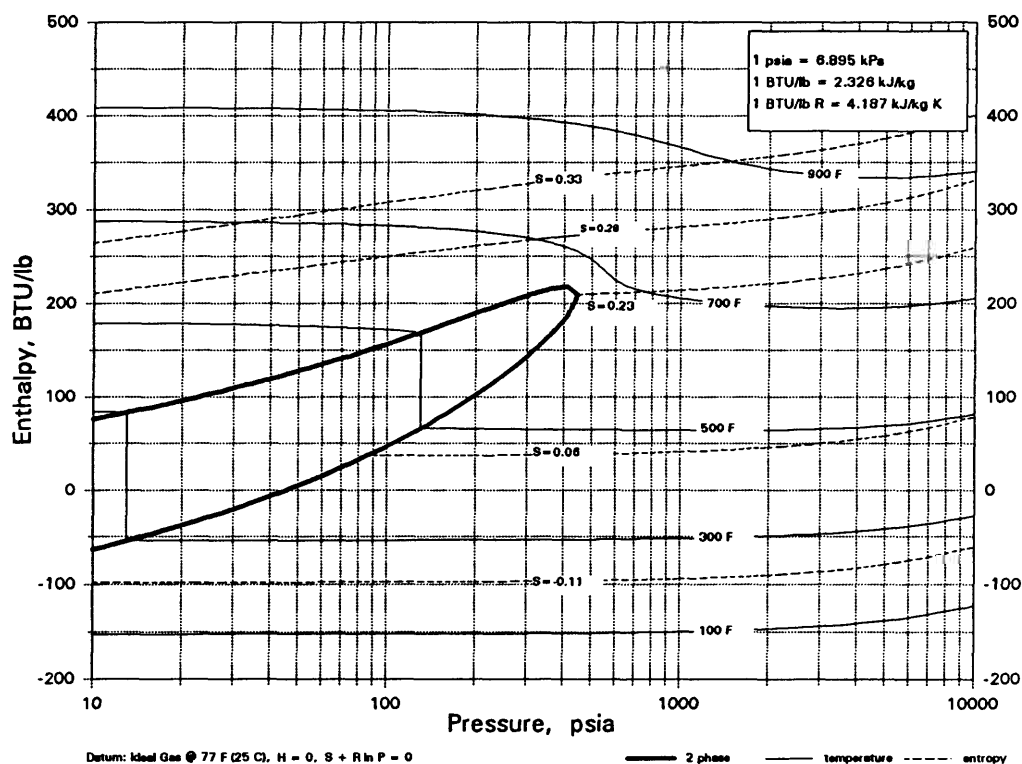
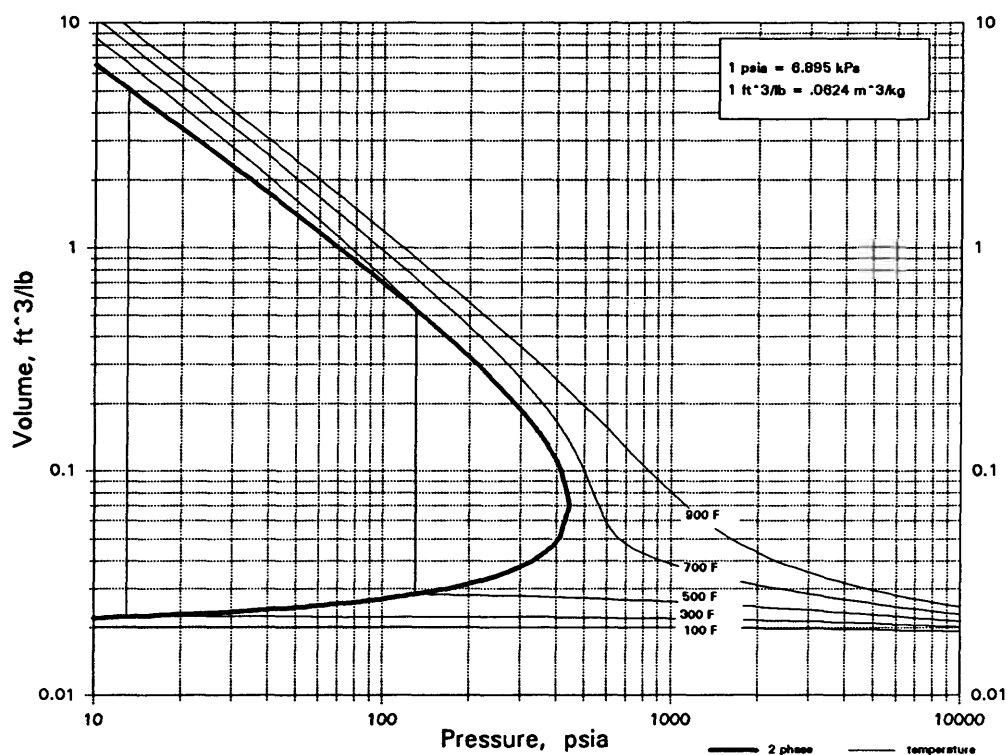
C6H14O6

SORBITOL



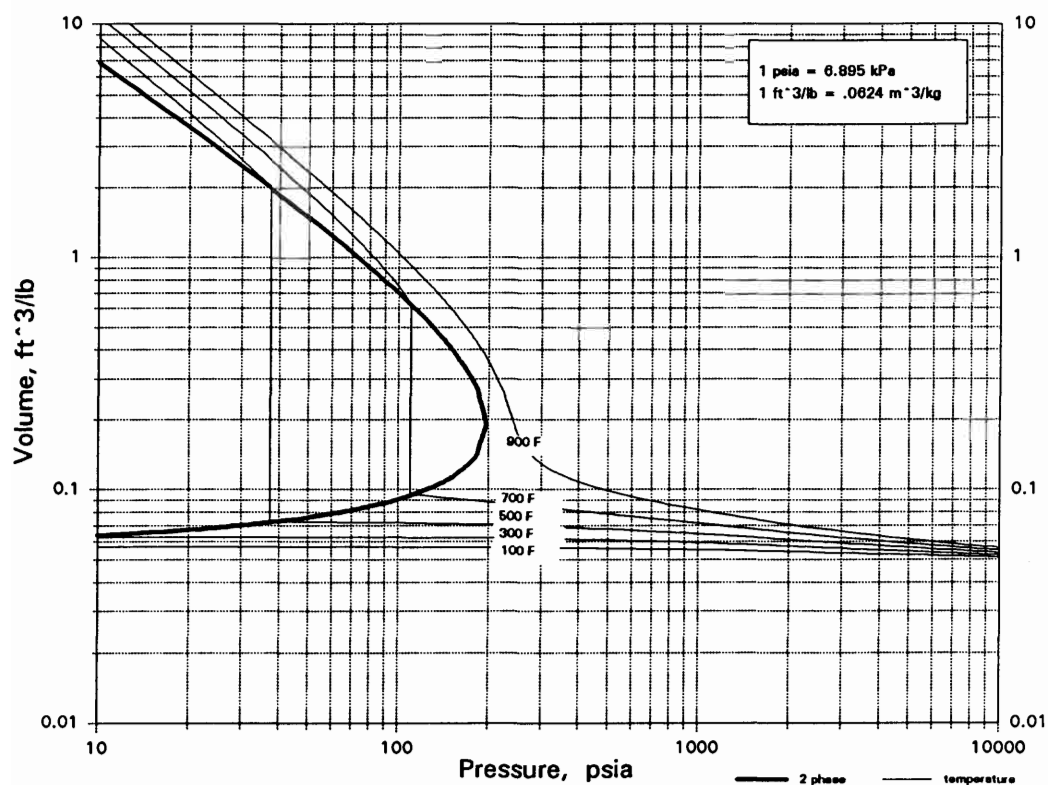
C6H14S

n-HEXYLMERCAPTAN



C6H15Al

TRIETHYL ALUMINIUM



1. Boiling Point, K..... 458.15

2. Critical Temperature, K.... 720.15

3. Critical Pressure, atm..... 13.40

Heat capacity data are not available.

C₆H₁₅Al₂Cl₃	ETHYL ALUMINUM SESQUICHLORIDE
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1. Molecular Weight, lb/mol..... 247.51

2. Boiling Point, K..... 482.15

Critical data (T_c, P_c) are not available.

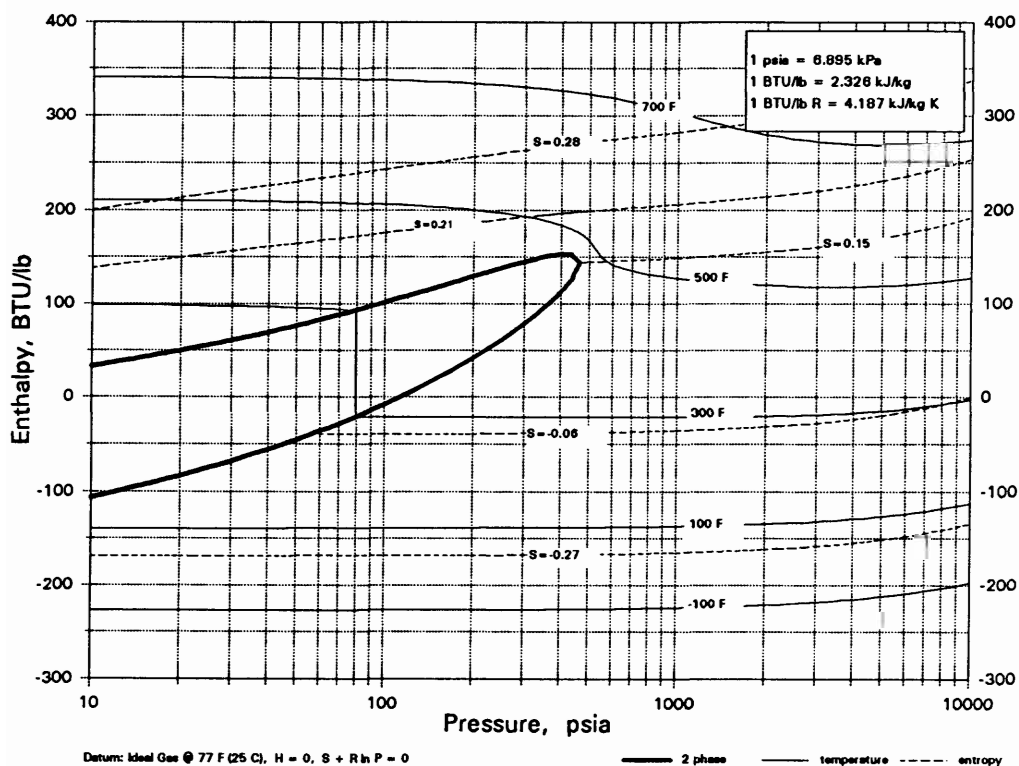
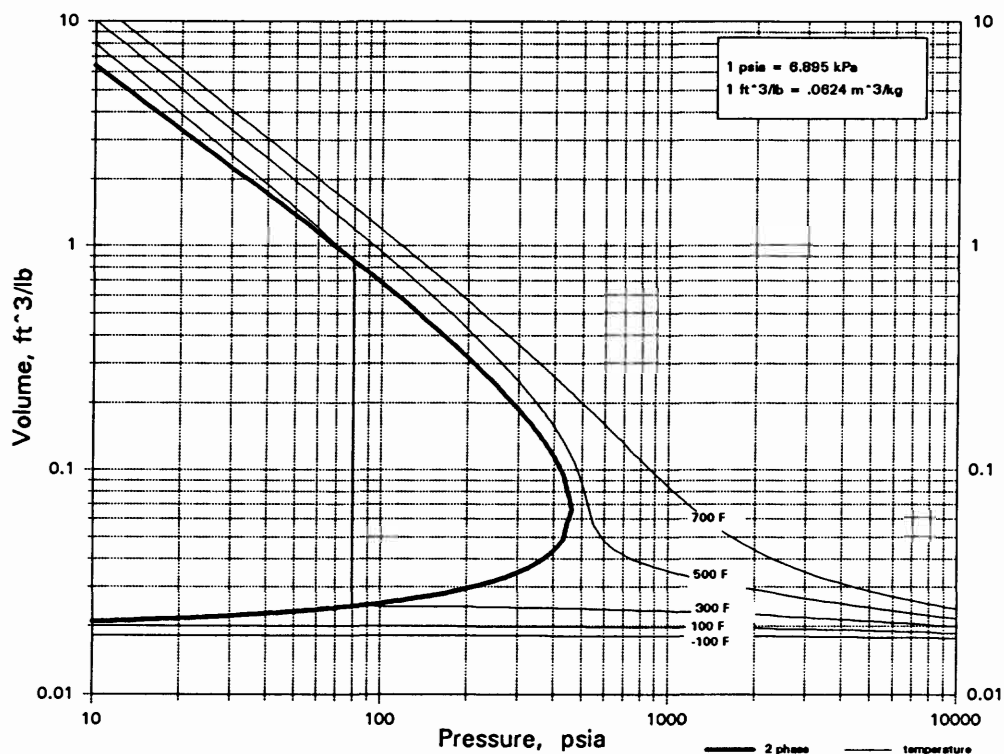
1. Molecular Weight, lb/mol..... 247.51

2. Boiling Point, K..... 482.15

Critical data (T_c, P_c) are not available.

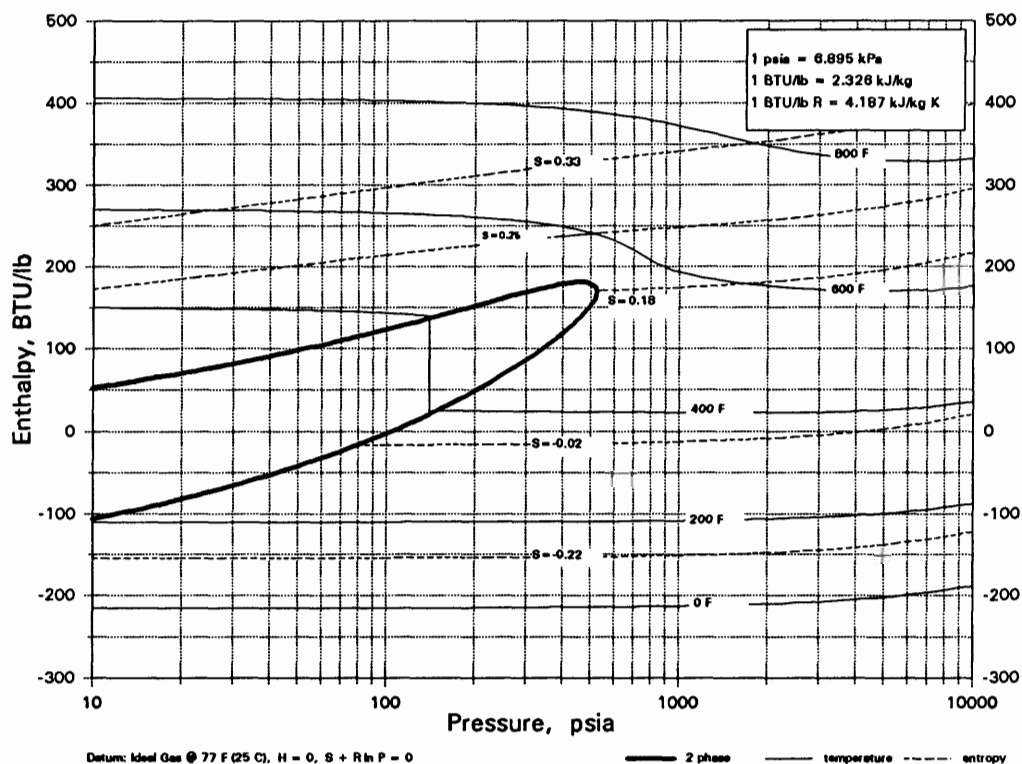
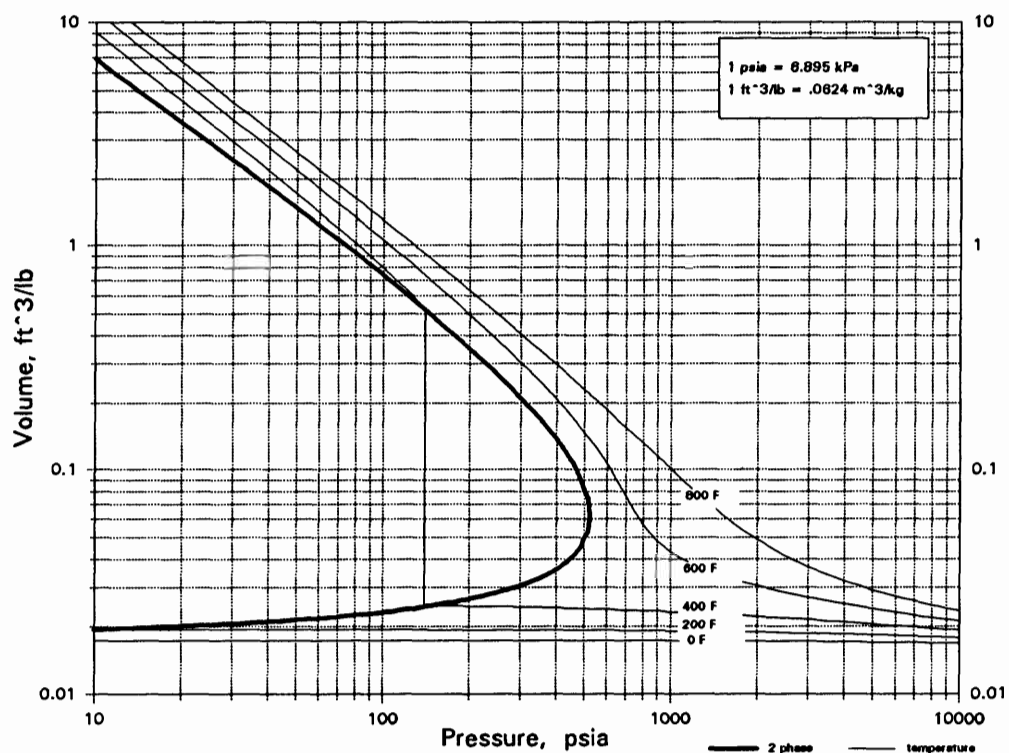
C6H15N

DIISOPROPYLAMINE

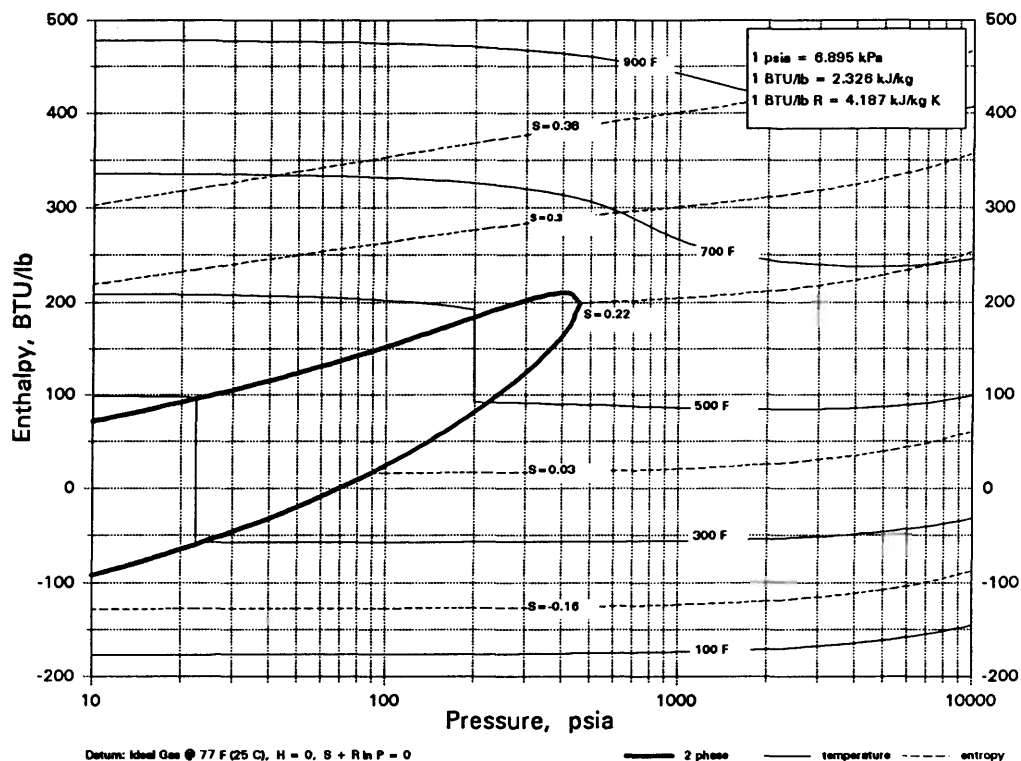
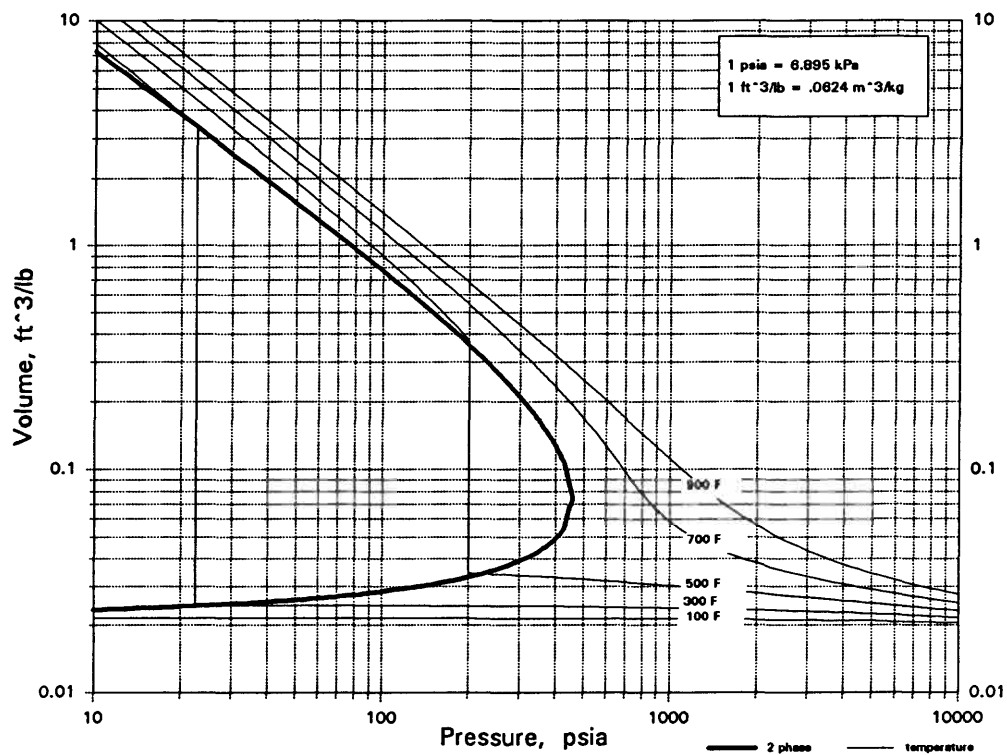


C6H15N

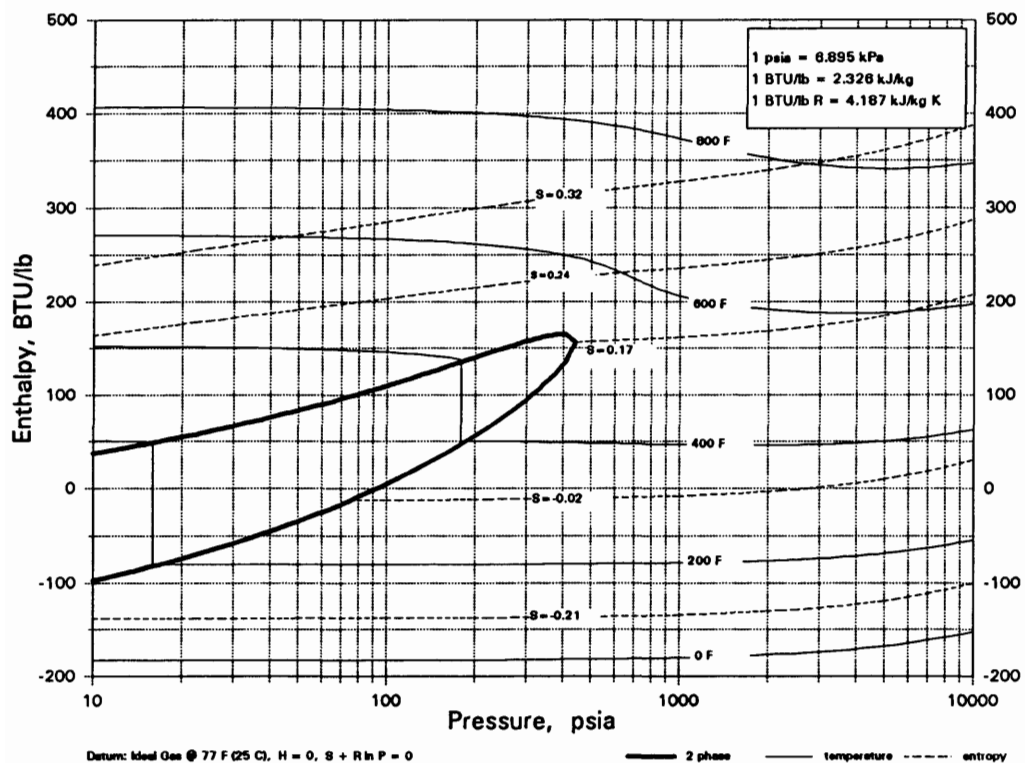
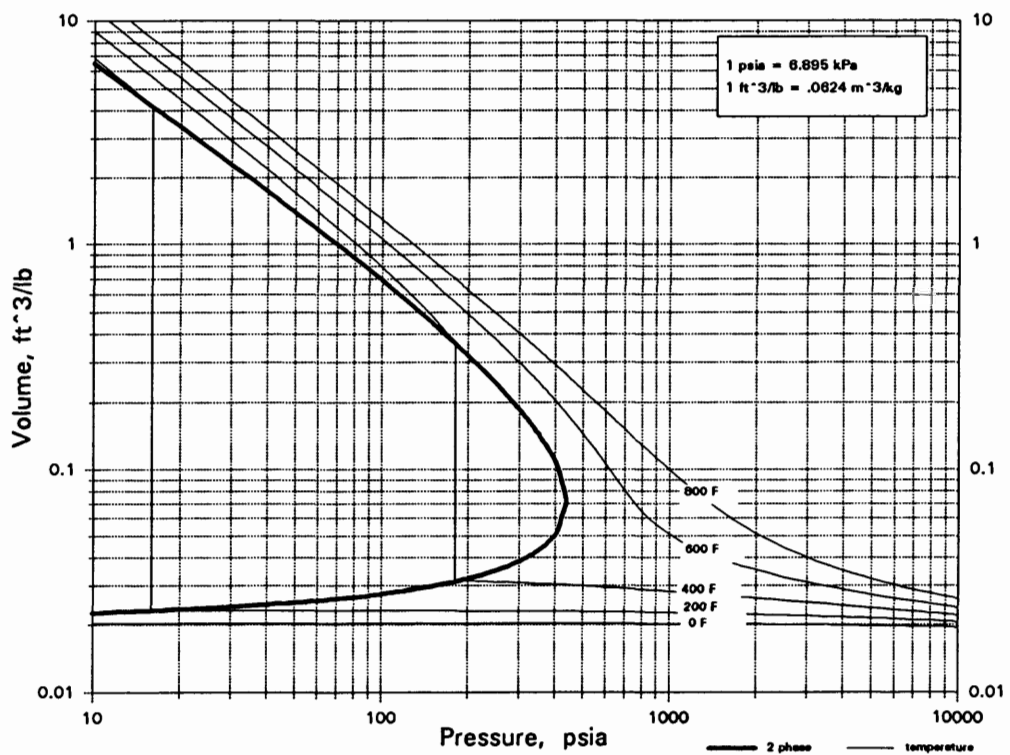
DI-n-PROPYLAMINE



C6H15N
n-HEXYLAMINE

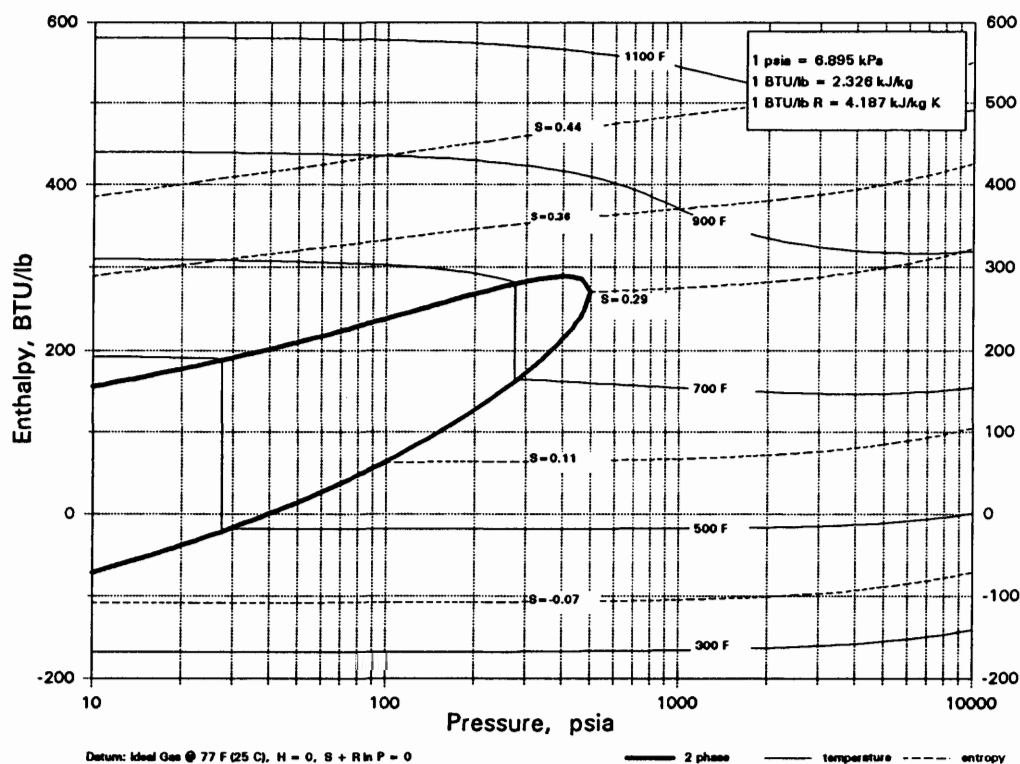
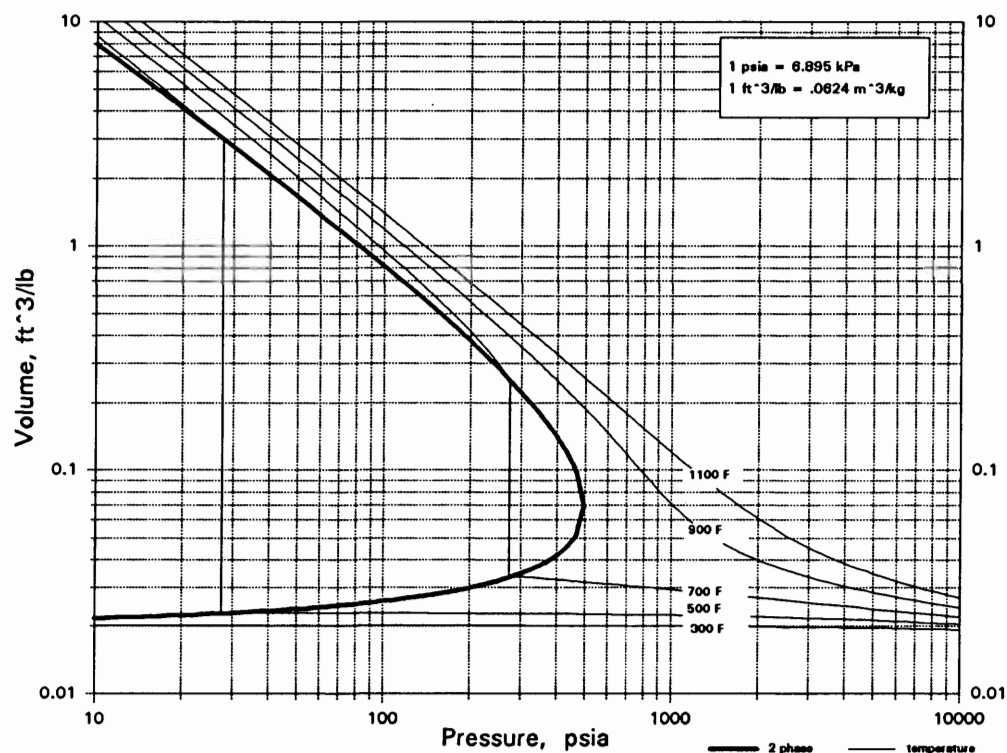


C6H15N
TRIETHYLAMINE



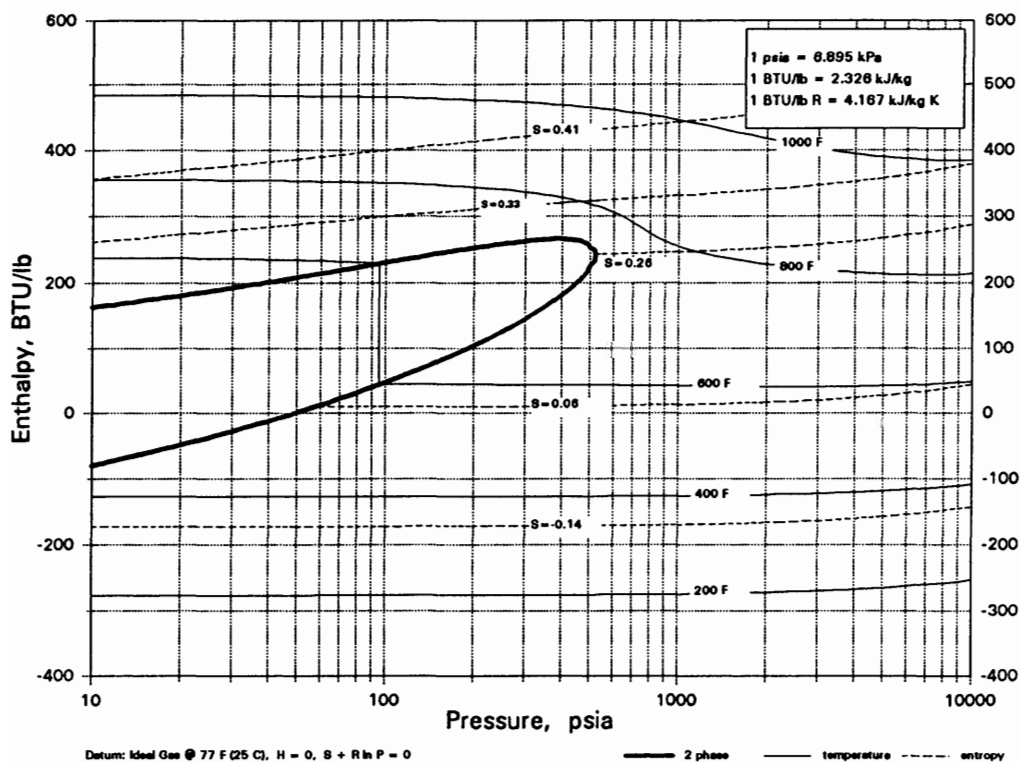
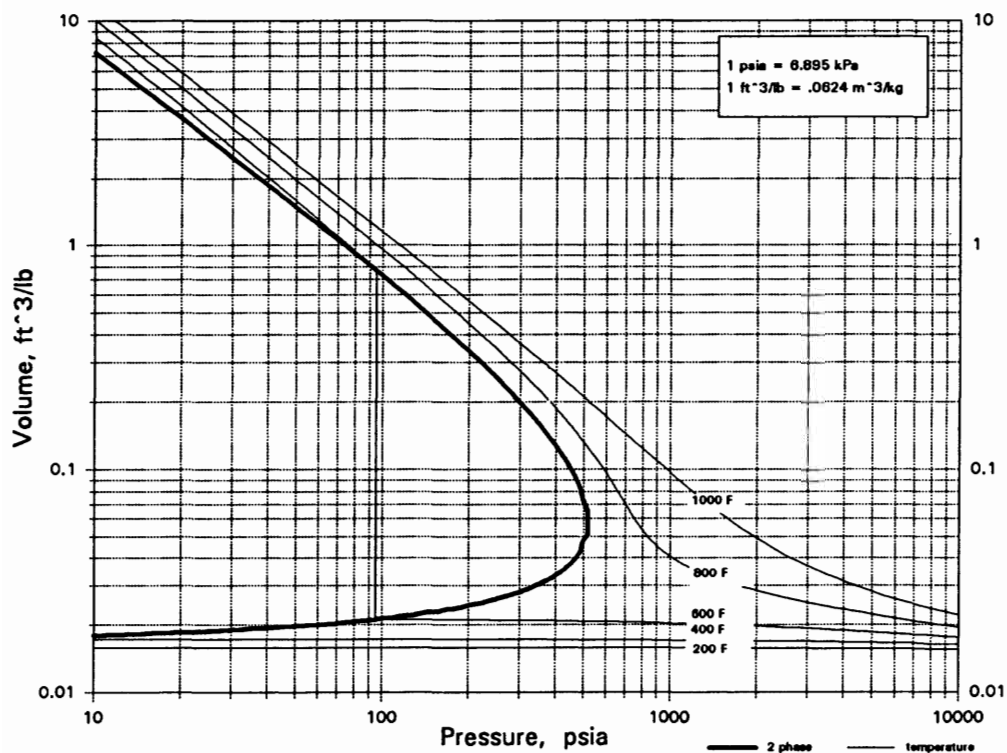
C6H15NO

6-AMINOHEXANOL

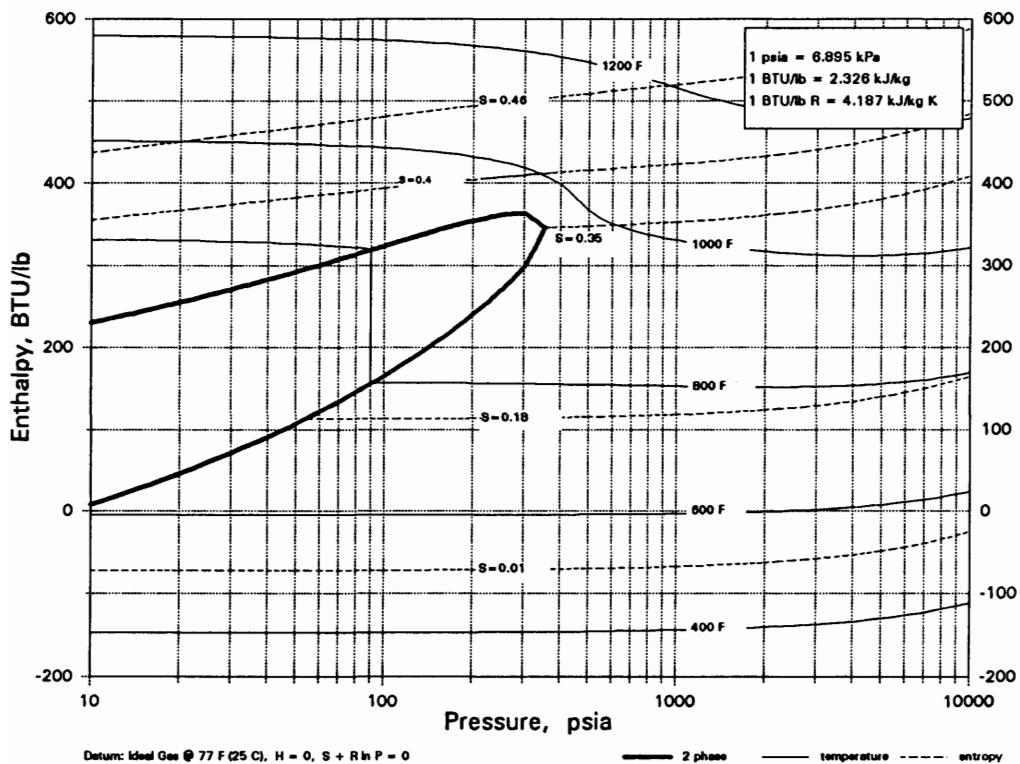
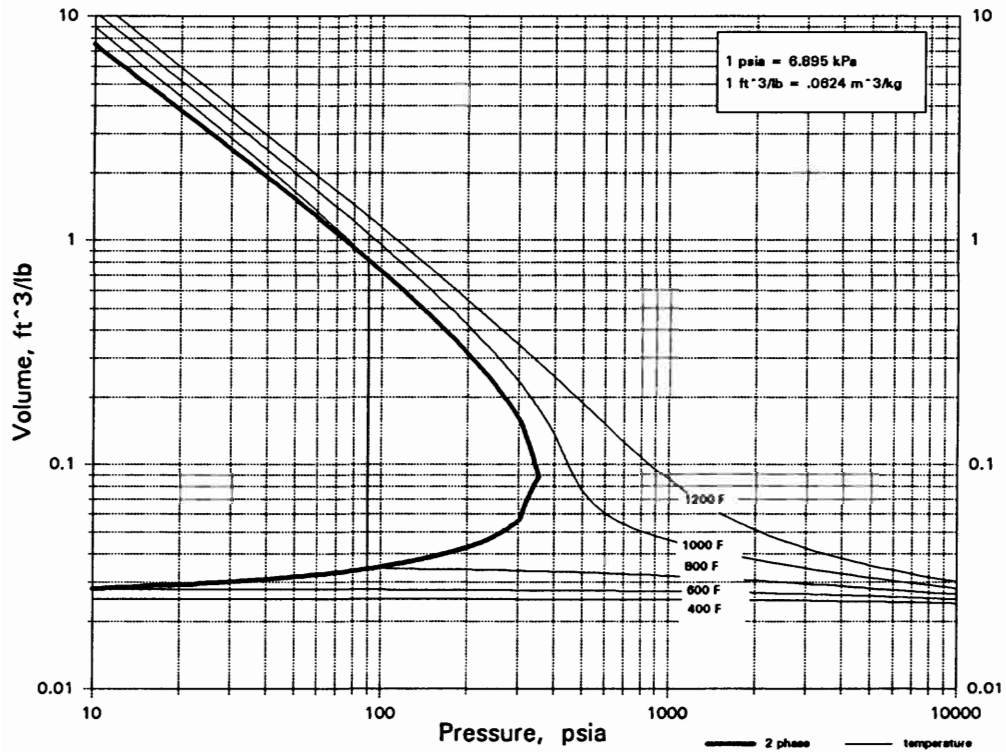


C6H15NO2

DIISOPROPANOLAMINE

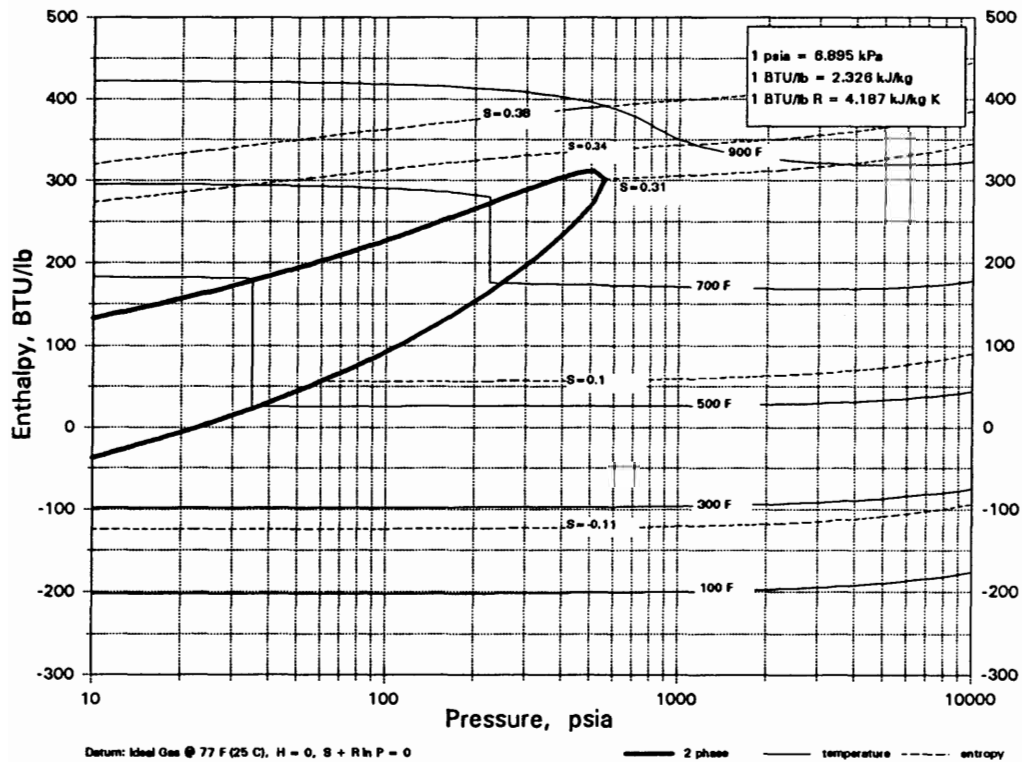
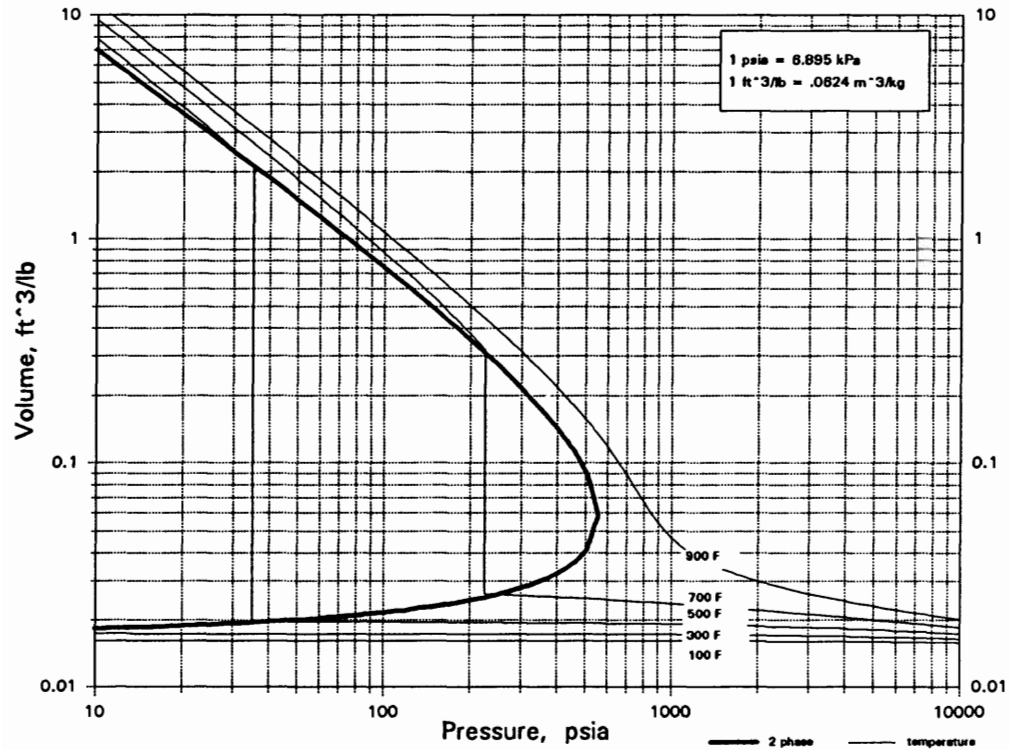


C6H15NO3 TRIETHANOLAMINE



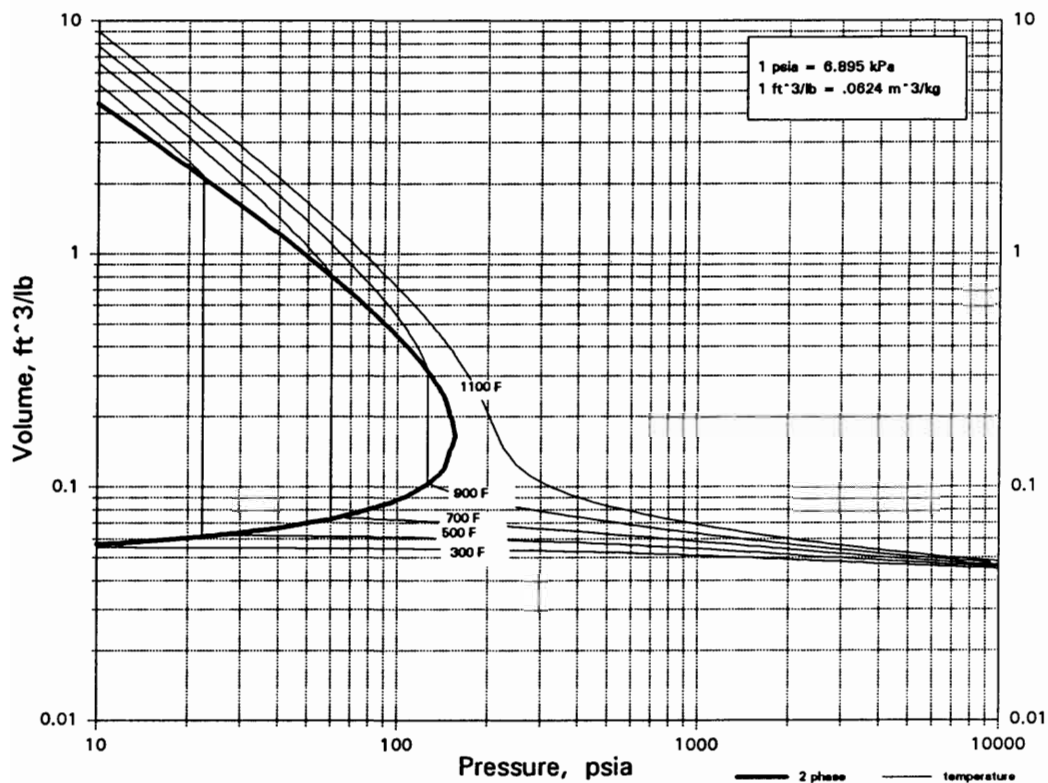
C6H15N3

N-AMINOETHYL PIPERAZINE



C6H15O4P

TRIETHYL PHOSPHATE



1. Boiling Point, K..... 484.15

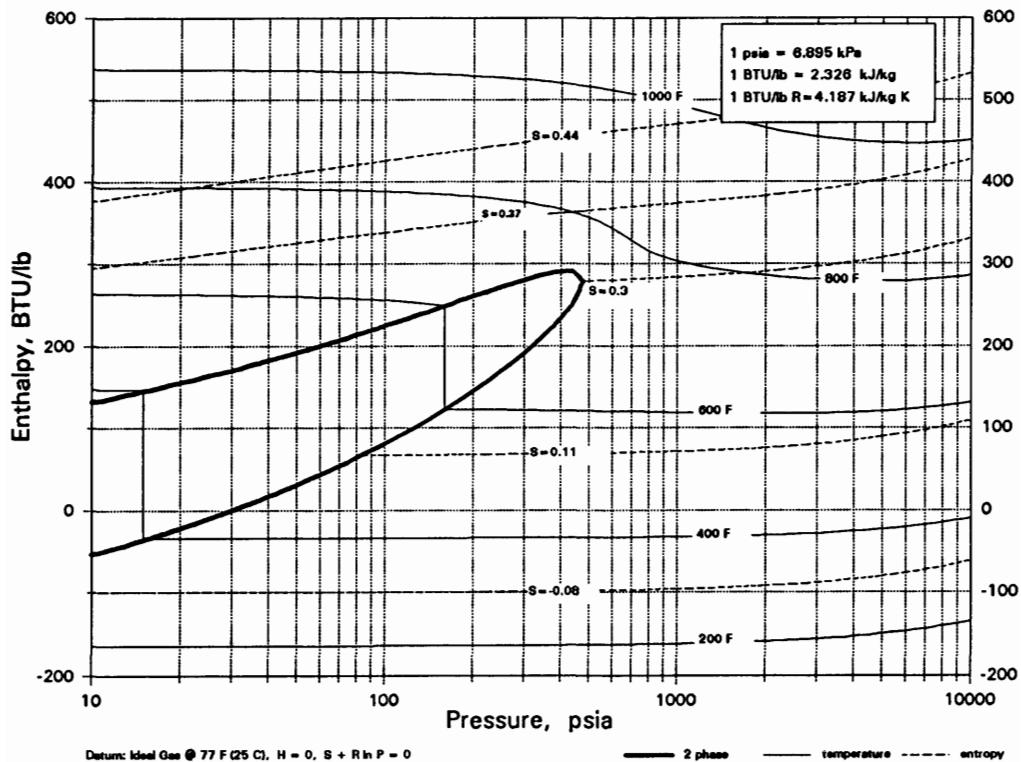
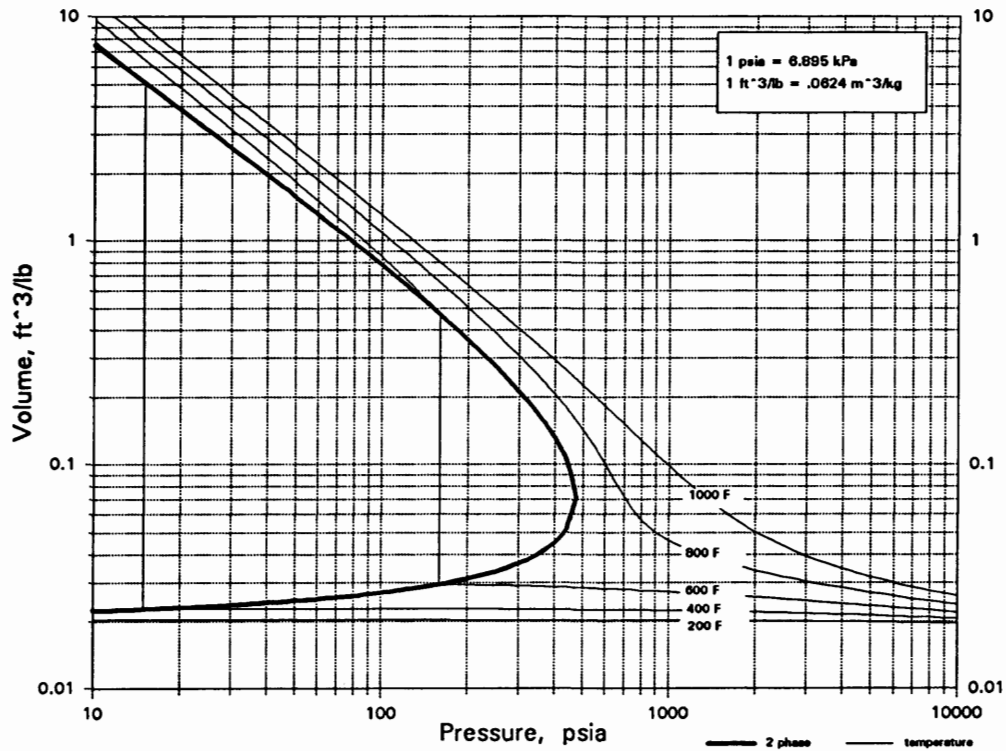
2. Critical Temperature, K.... 794.00

3. Critical Pressure, atm..... 10.66

Heat capacity data are not available.

C6H16N2

HEXAMETHYLENEDIAMINE



C6H18N3OP	HEXAMETHYL PHOSPHORAMIDE
------------------	---------------------------------

1. Molecular Weight, lb/mol..... 179.20

2. Boiling Point, K..... 506.15

Critical data (Tc, Pc) are not available.

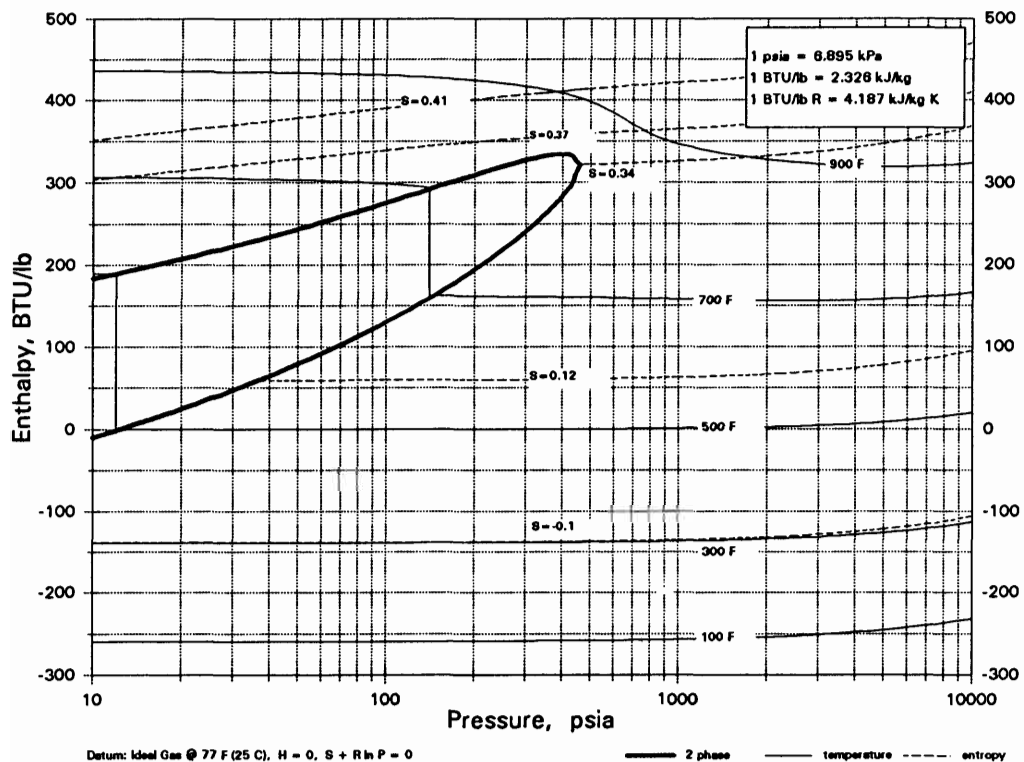
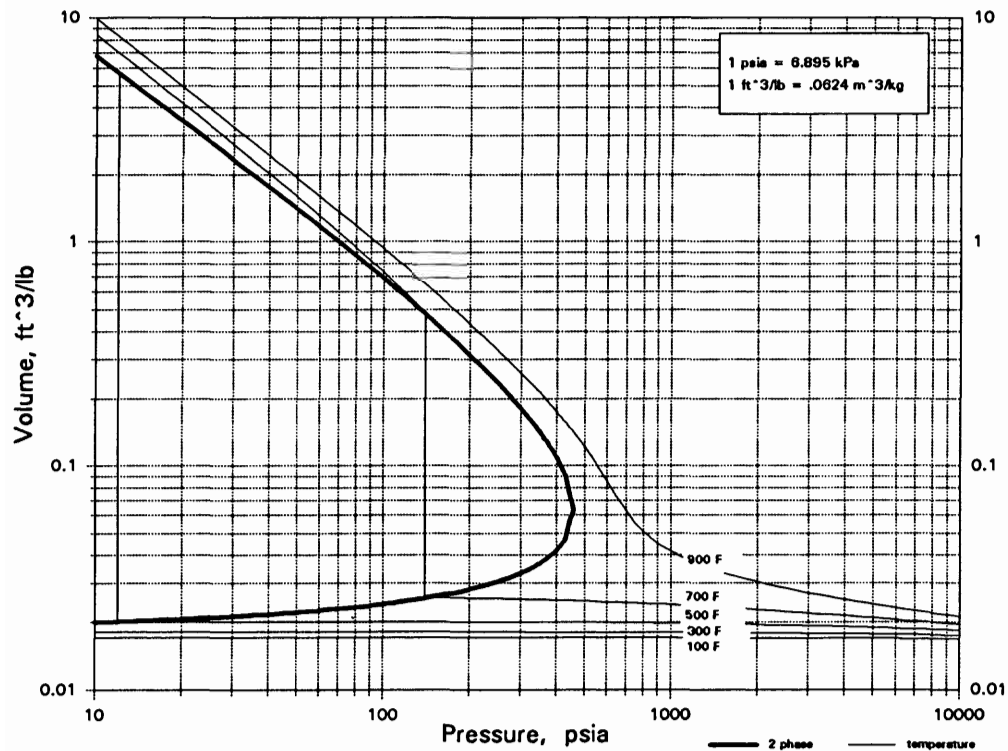
1. Molecular Weight, lb/mol..... 179.20

2. Boiling Point, K..... 506.15

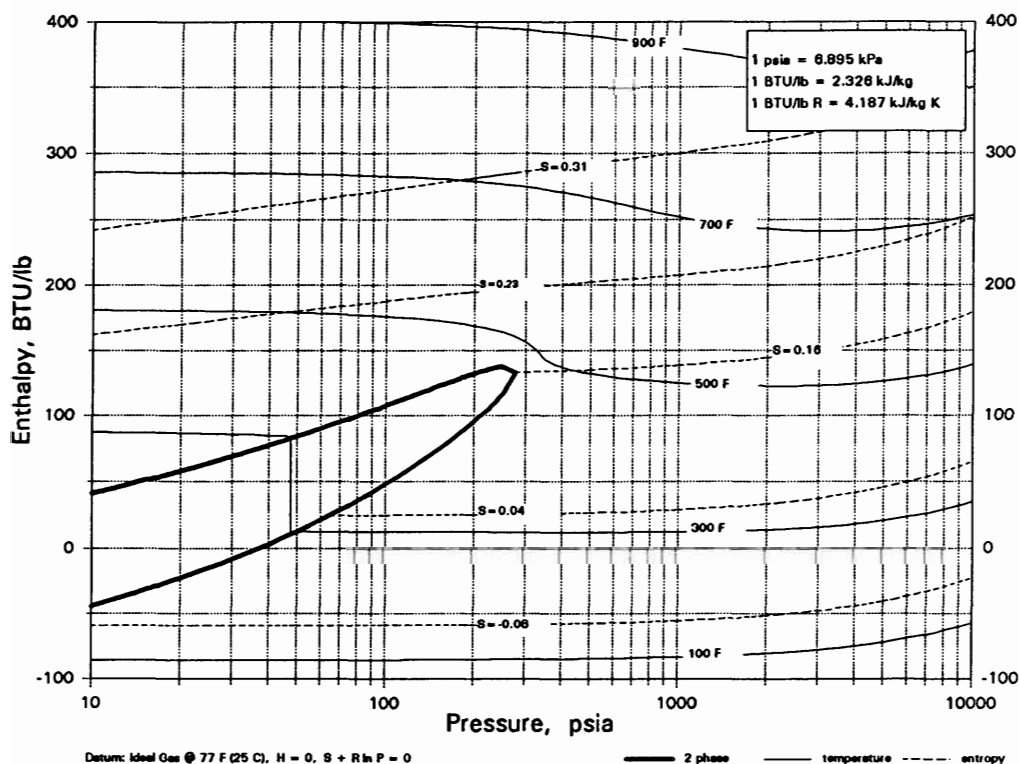
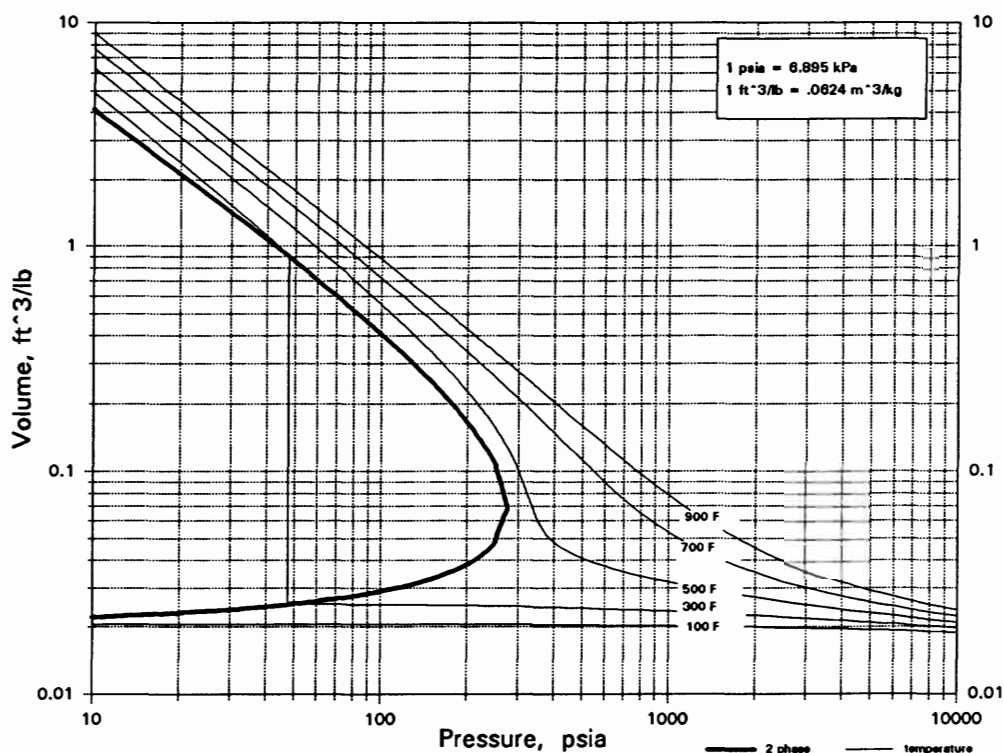
Critical data (Tc, Pc) are not available.

C6H18N4

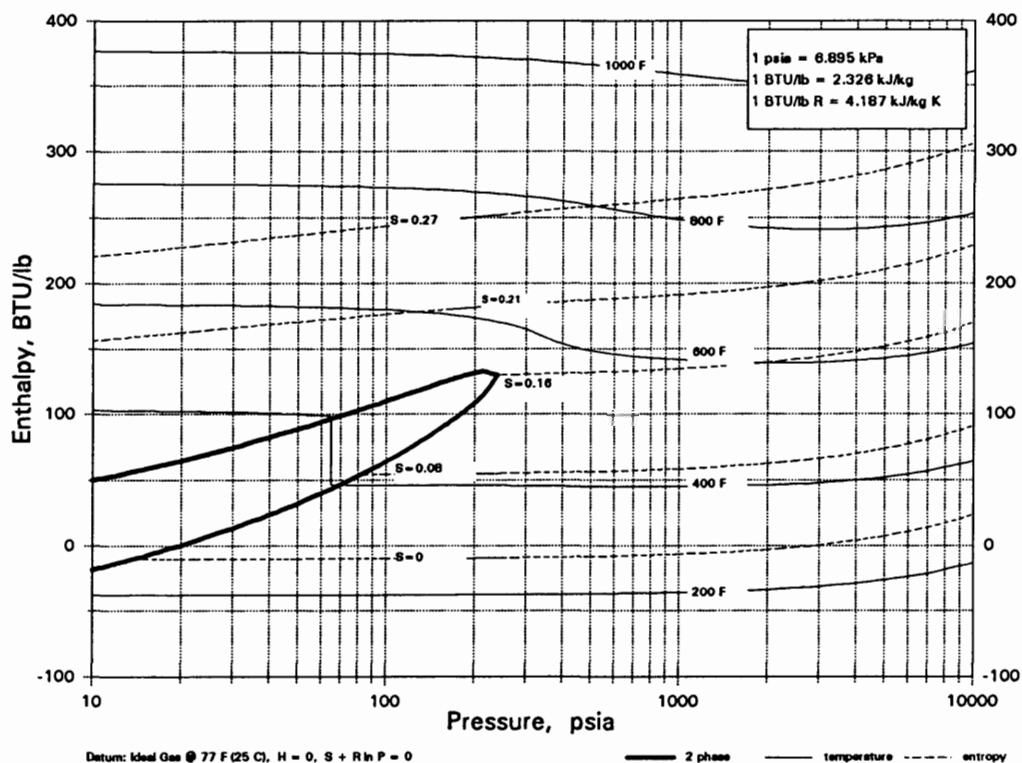
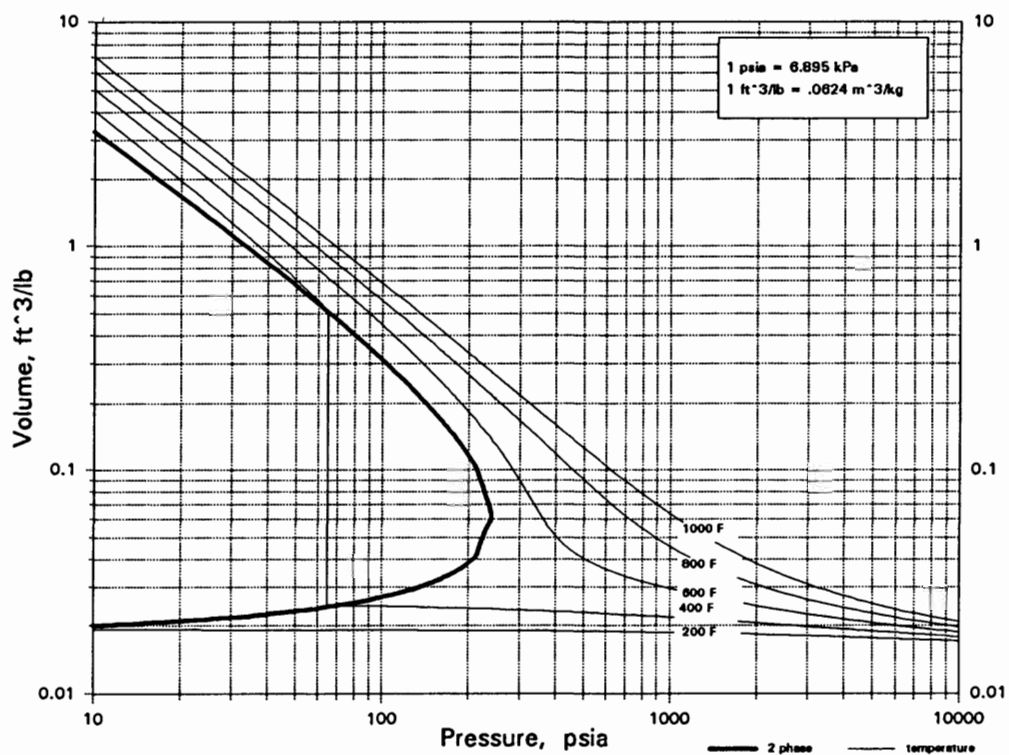
TRIETHYLENE TETRAMINE



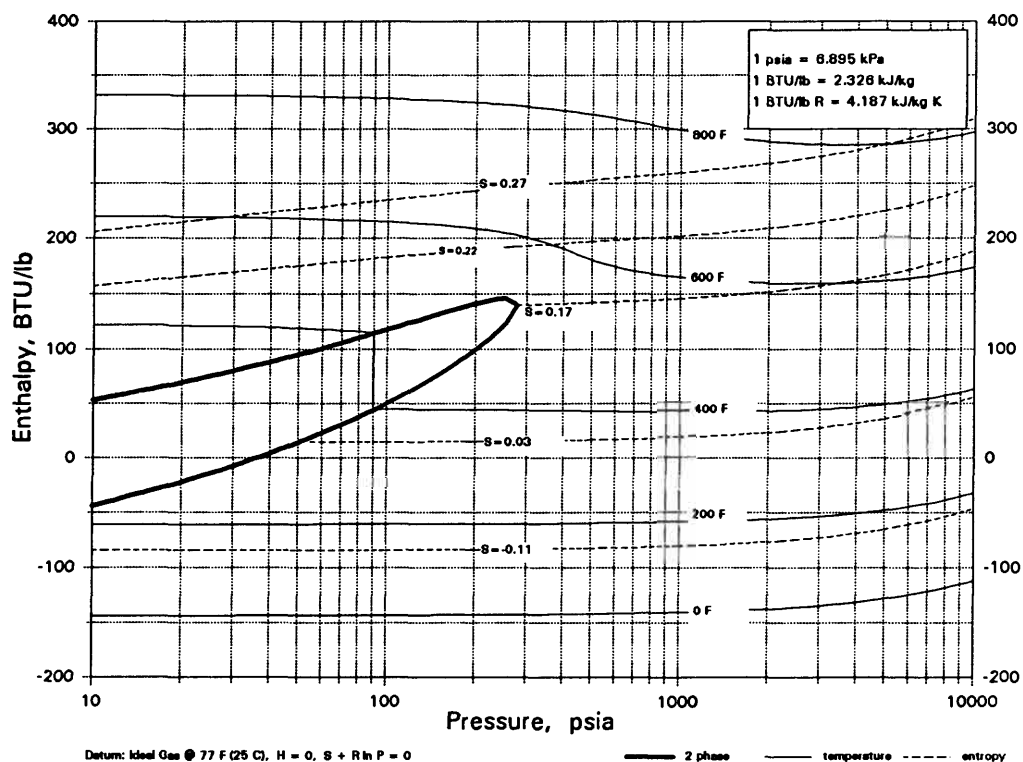
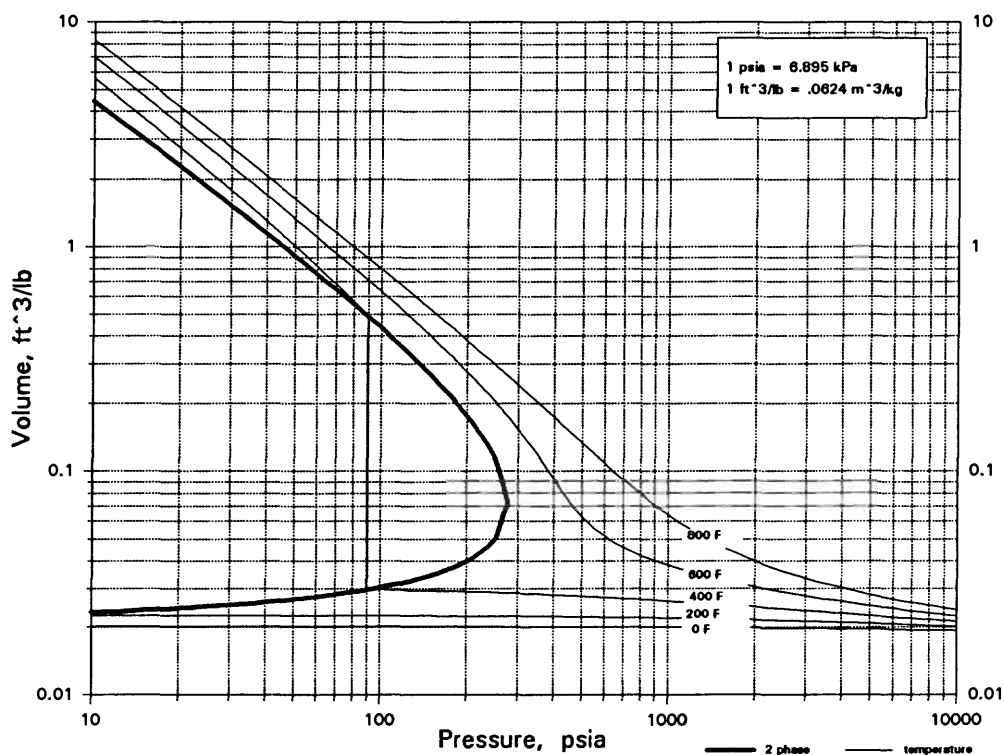
C6H18OSi2 HEXAMETHYLDISILOXANE



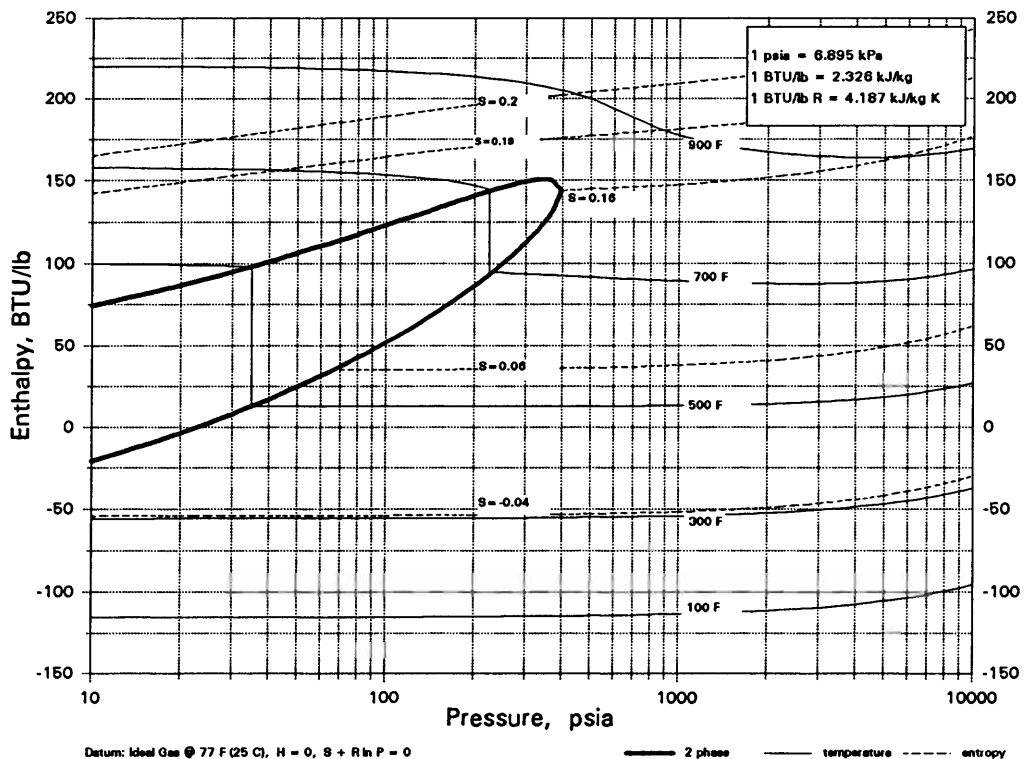
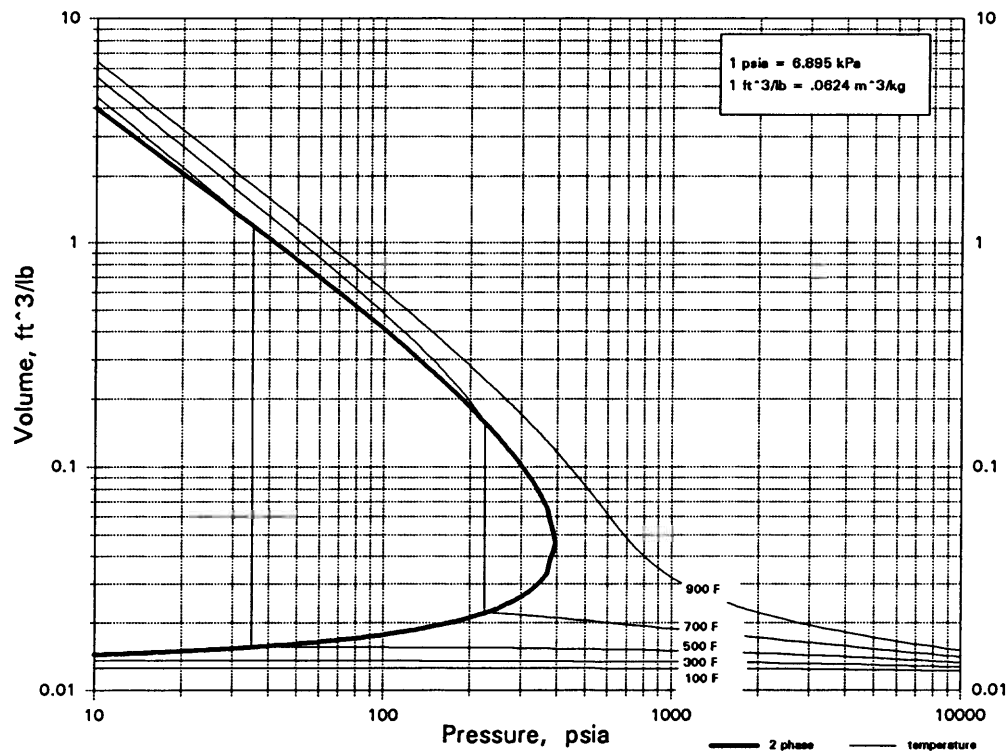
C6H18O3Si3 HEXAMETHYLCYCLOTRISILOXANE



C6H19NSi2 HEXAMETHYLDISILAZANE

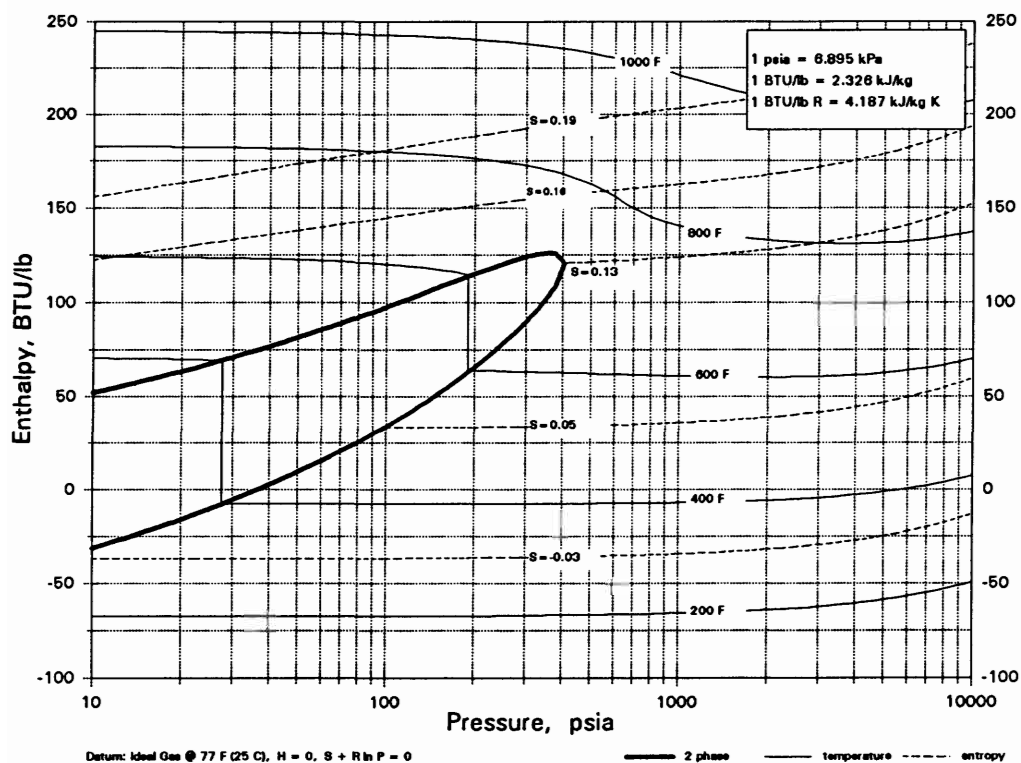
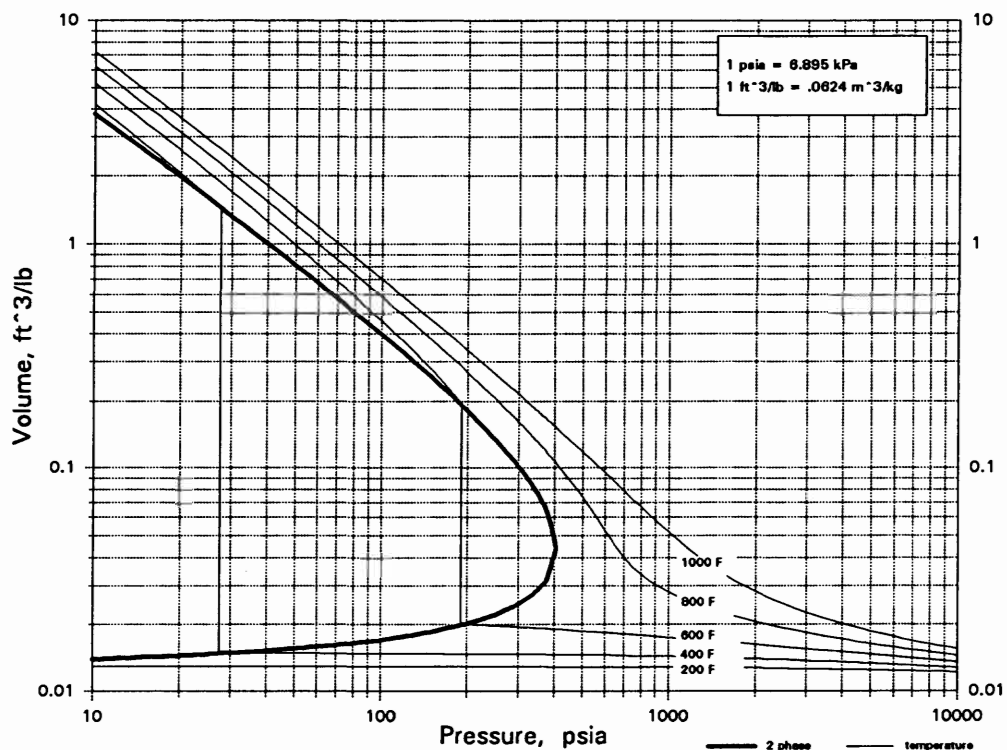


C7H3ClF3NO 24-CHLORO-3-NITROBENZOTRIFLUORIDE



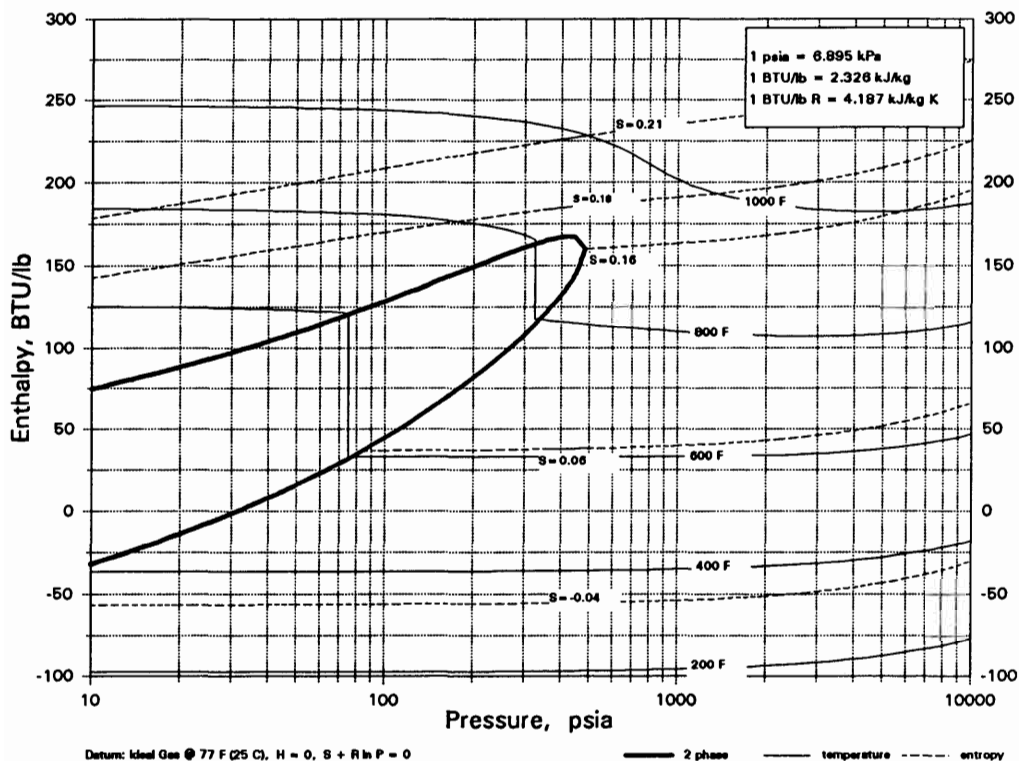
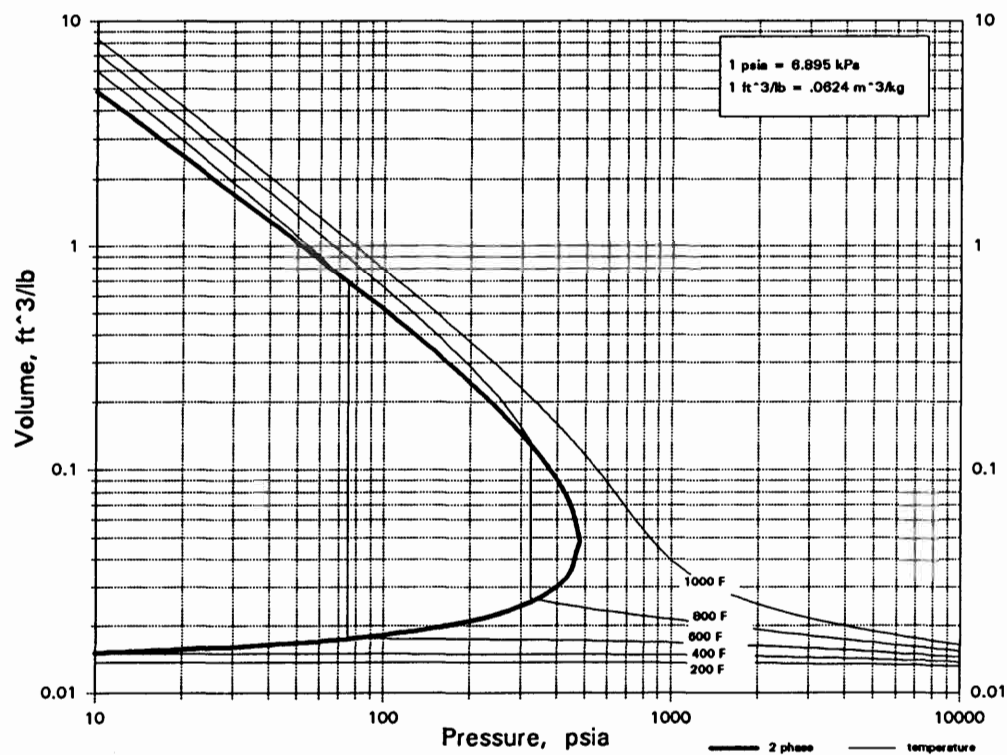
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2-4-DICHLOROBENZOTRIFLUORIDE



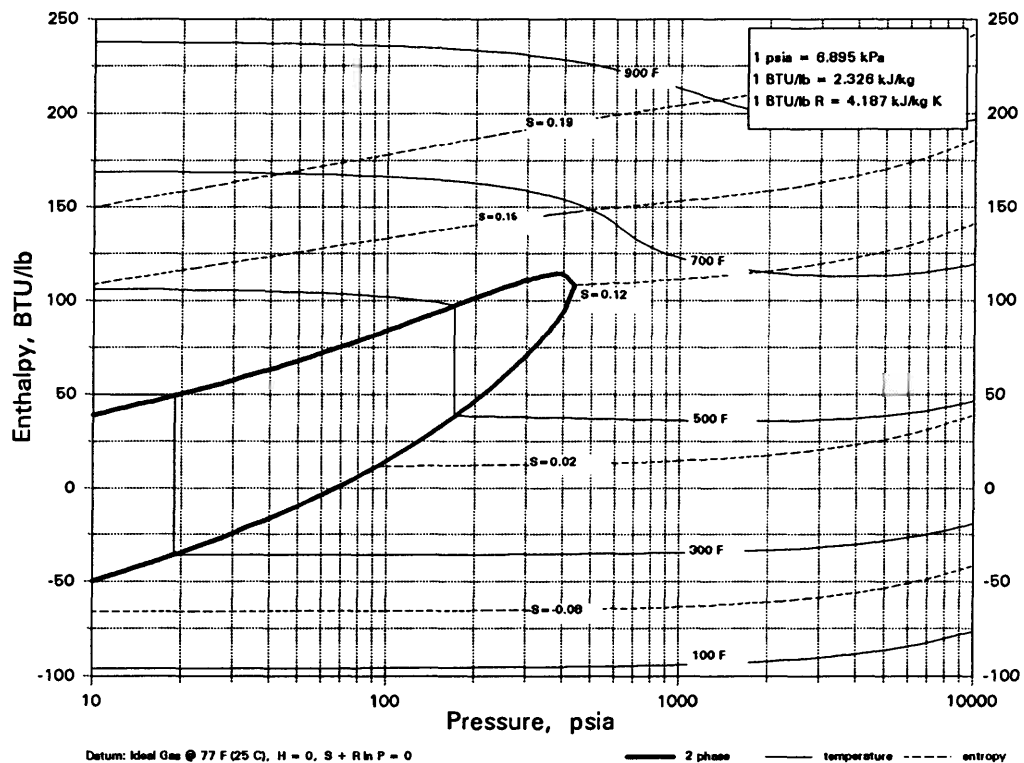
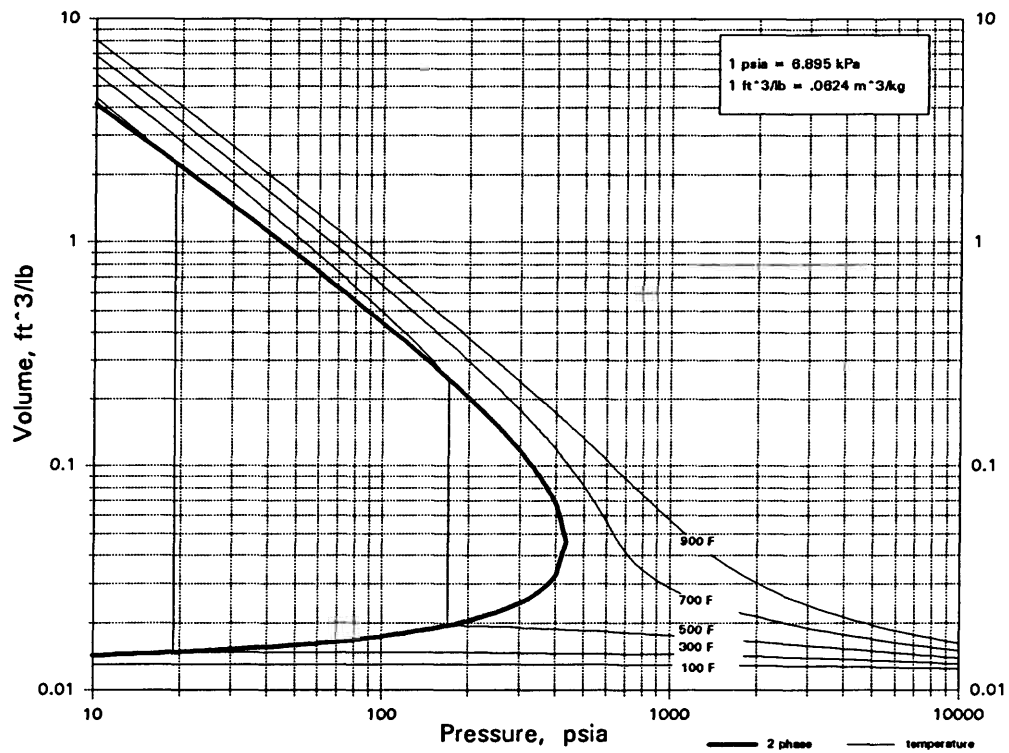
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3-4-DICHLOROPHENYL ISOCYANATE



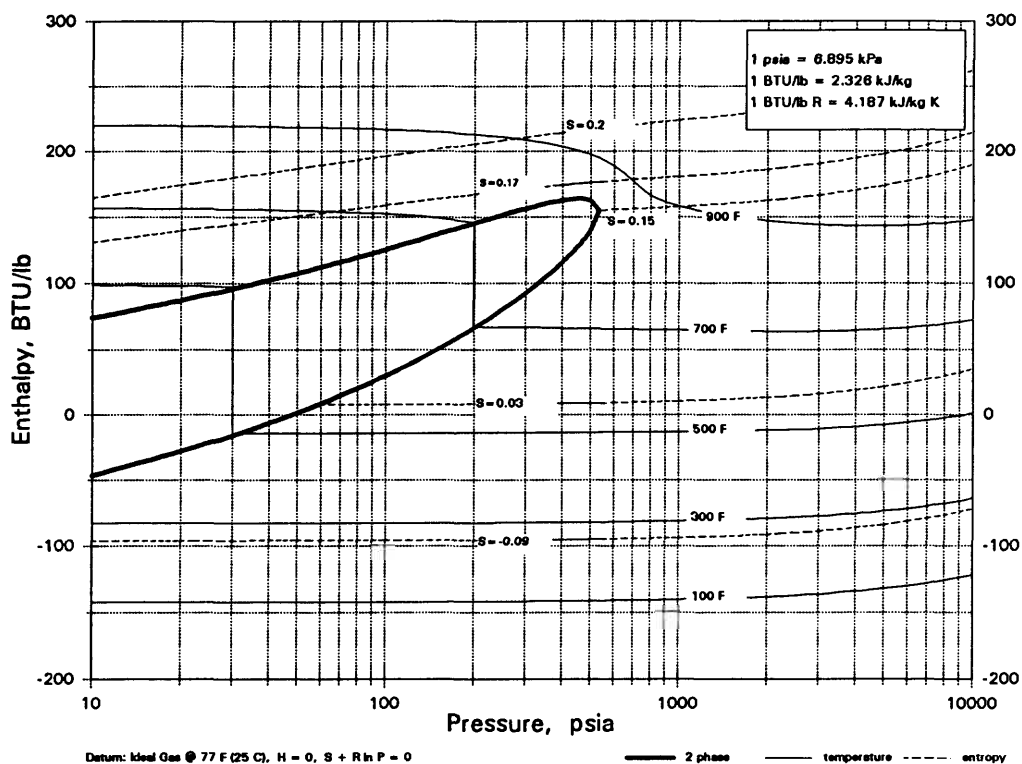
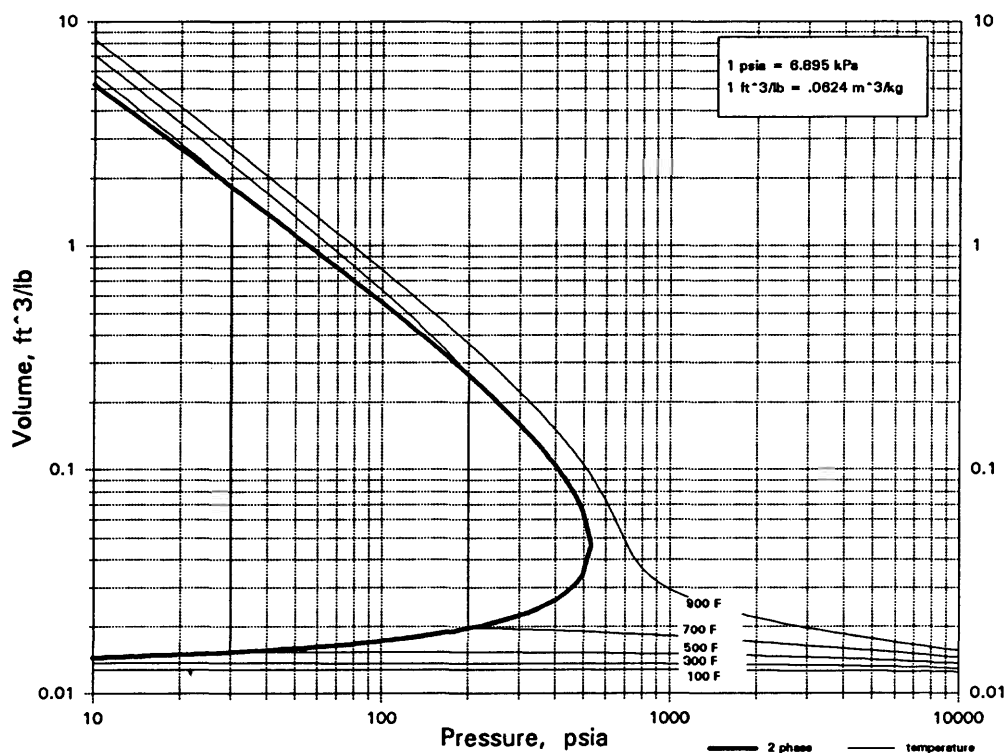
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p-CHLOROBENZOTRIFLUORIDE

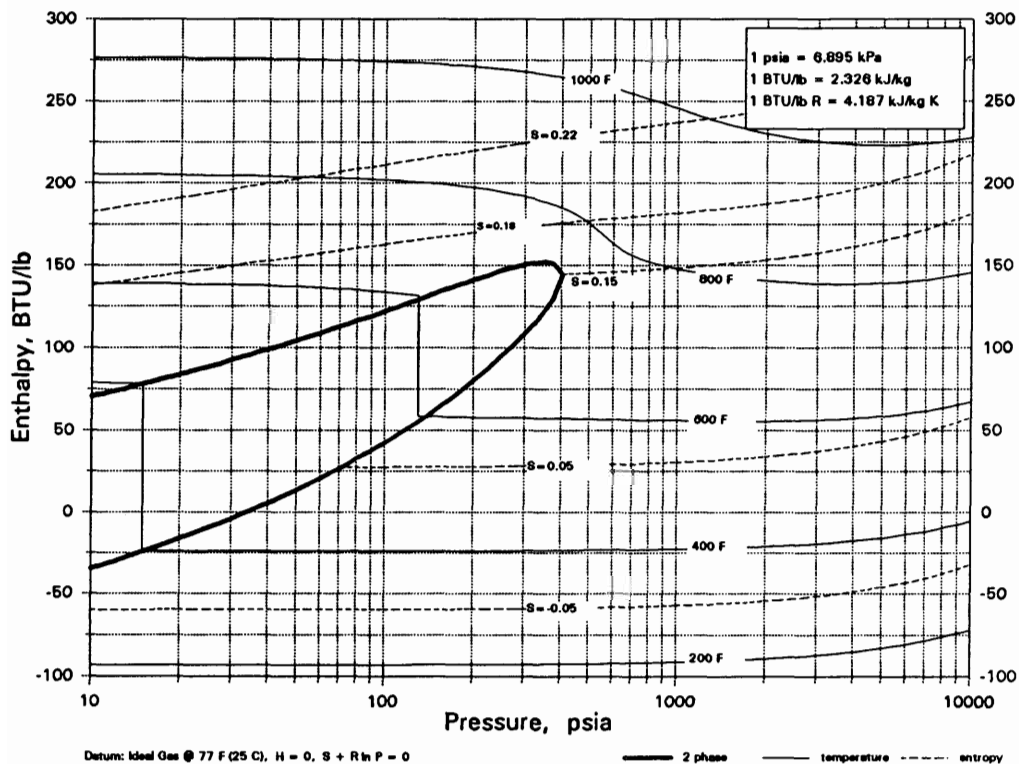
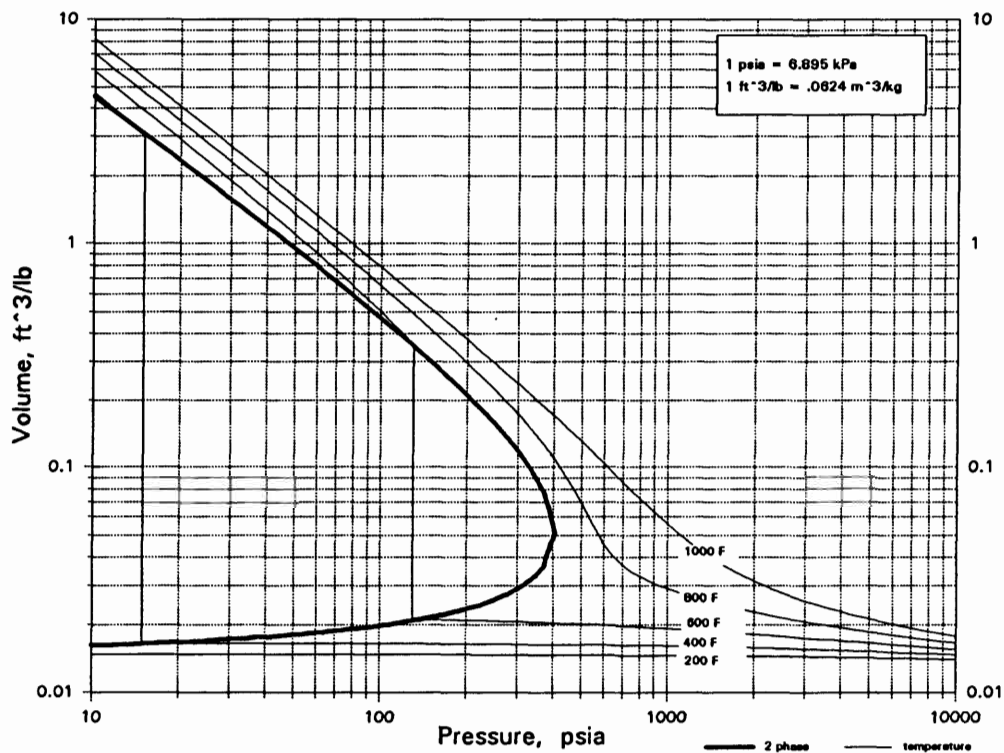


C7H4Cl2O

m-CHLOROBENZOYL CHLORIDE

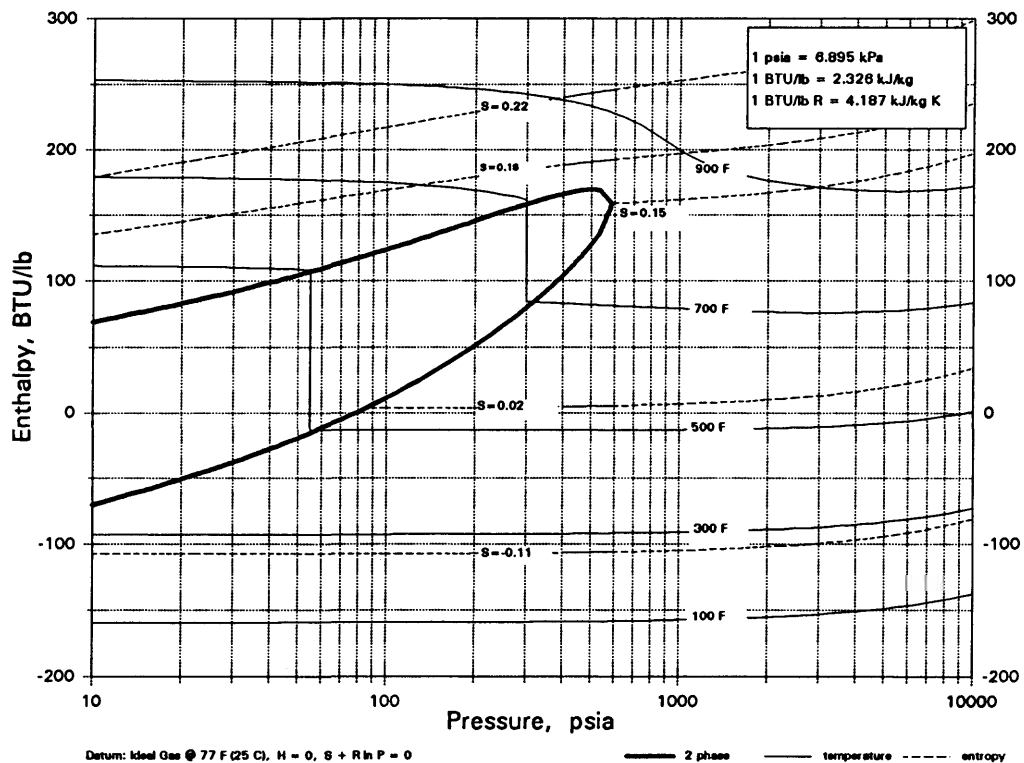
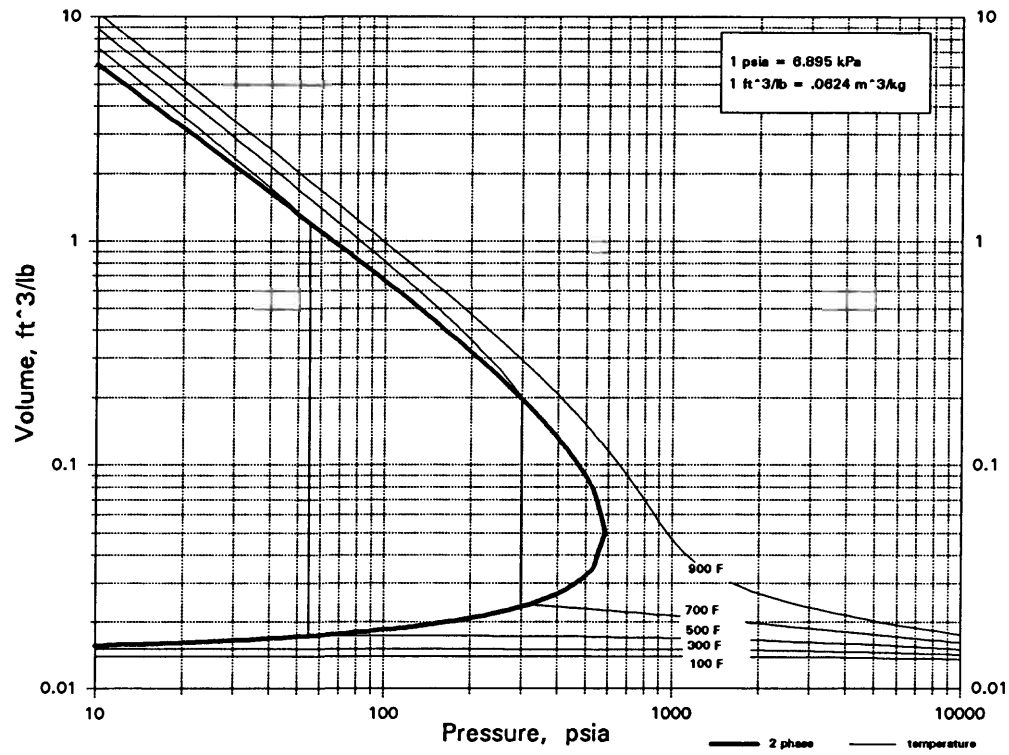


C7H4F3NO2 3-NITROBENZOTRIFLUORIDE

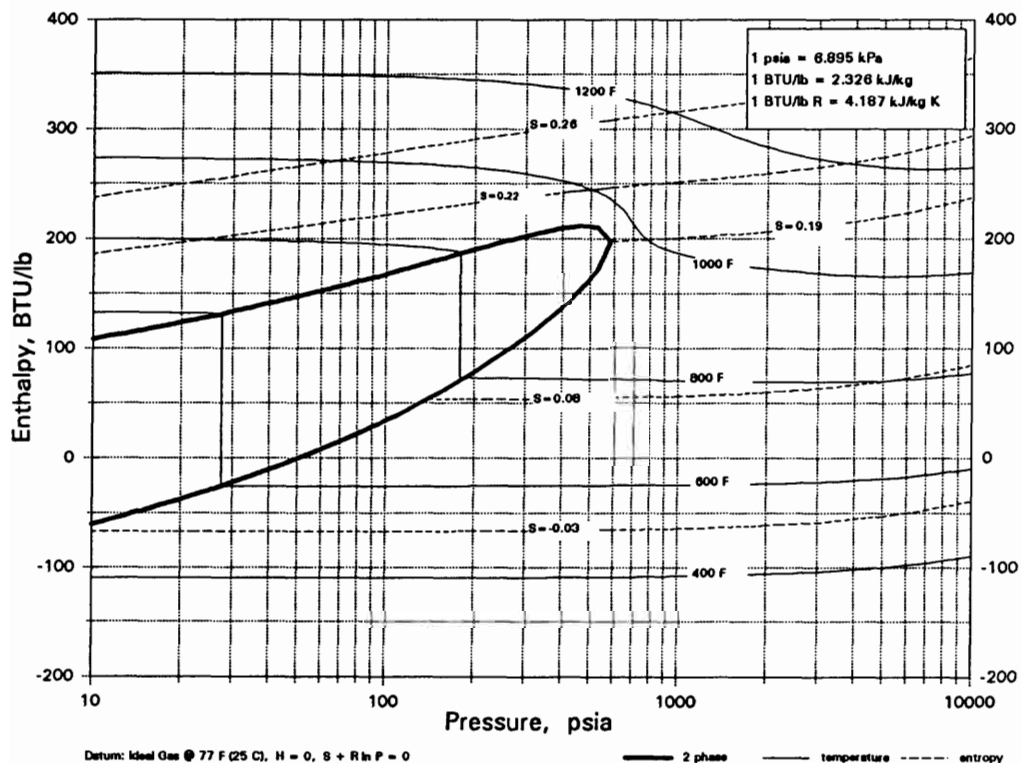
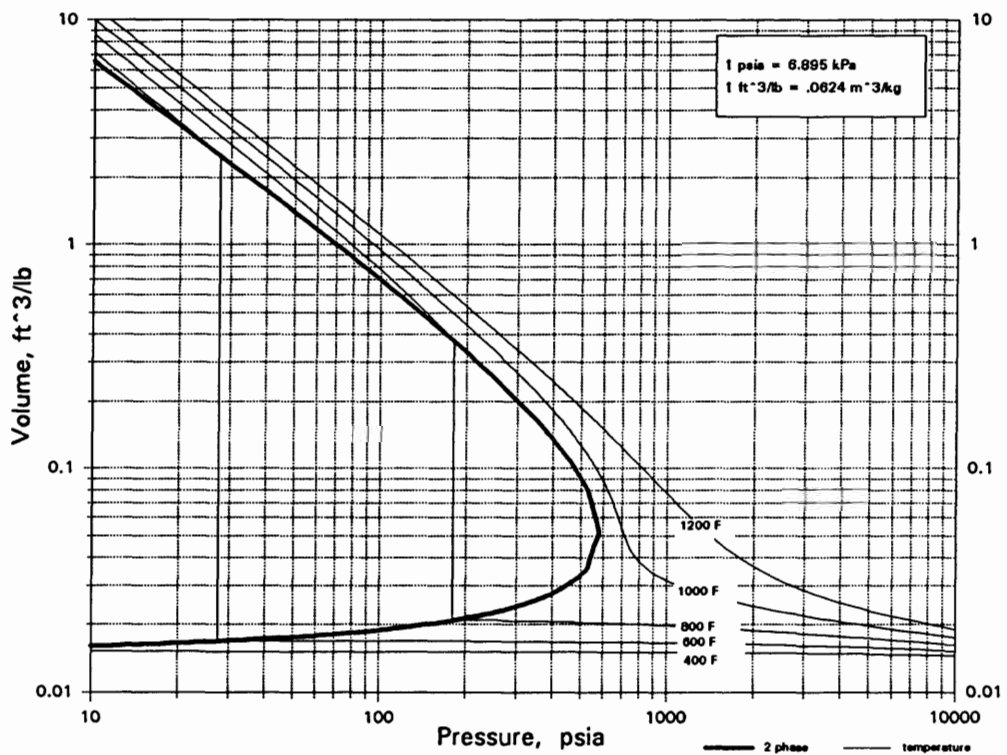


C7H5ClO

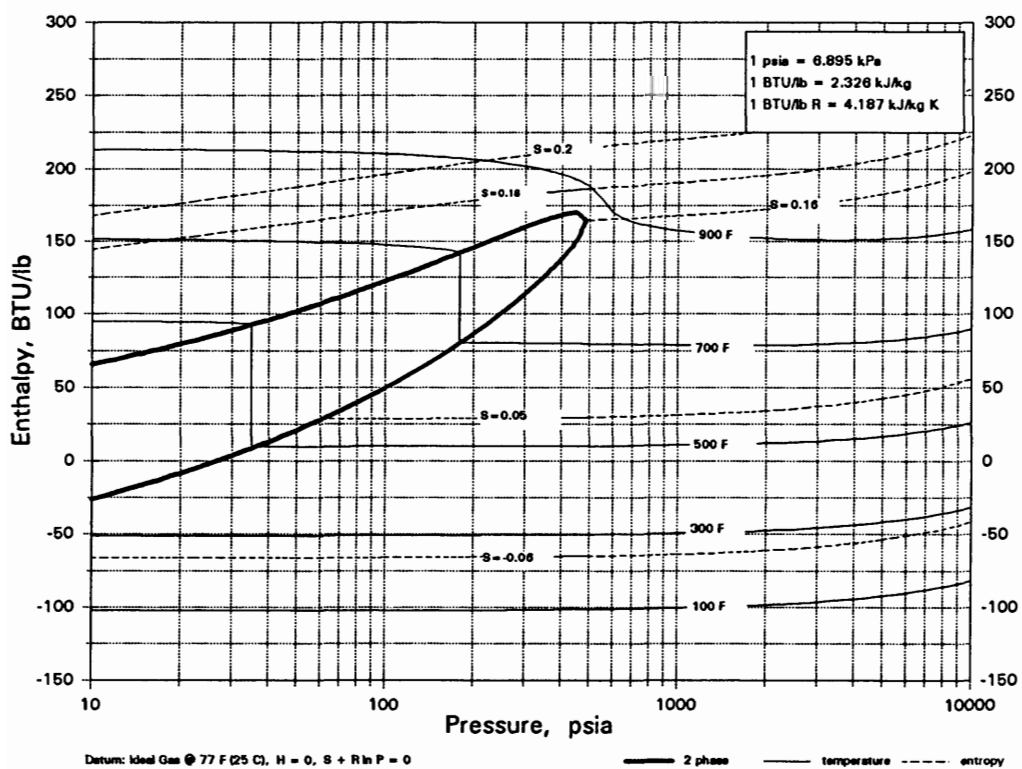
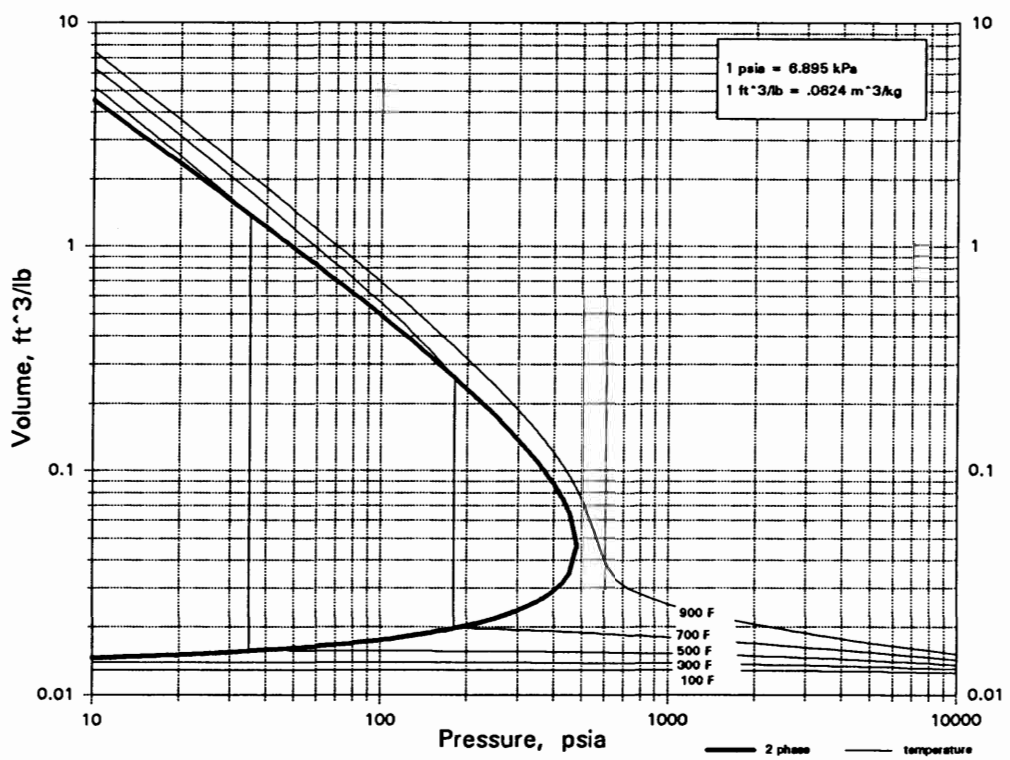
BENZOYL CHLORIDE



C7H5ClO2
o-CHLOROBENZOIC ACID

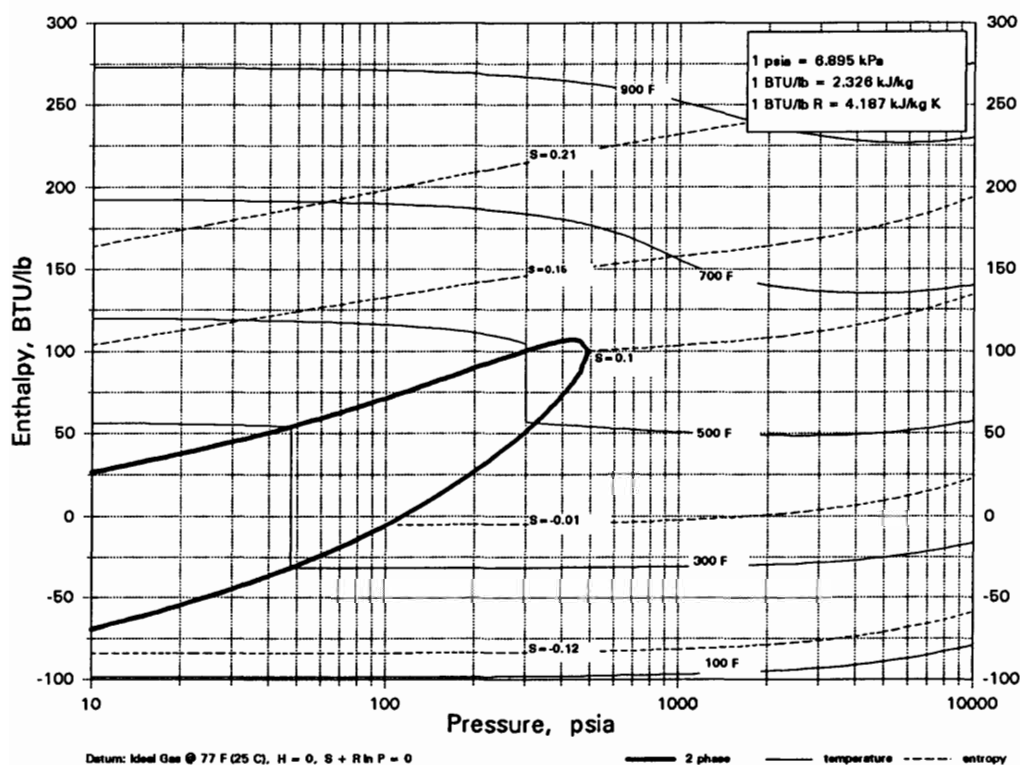
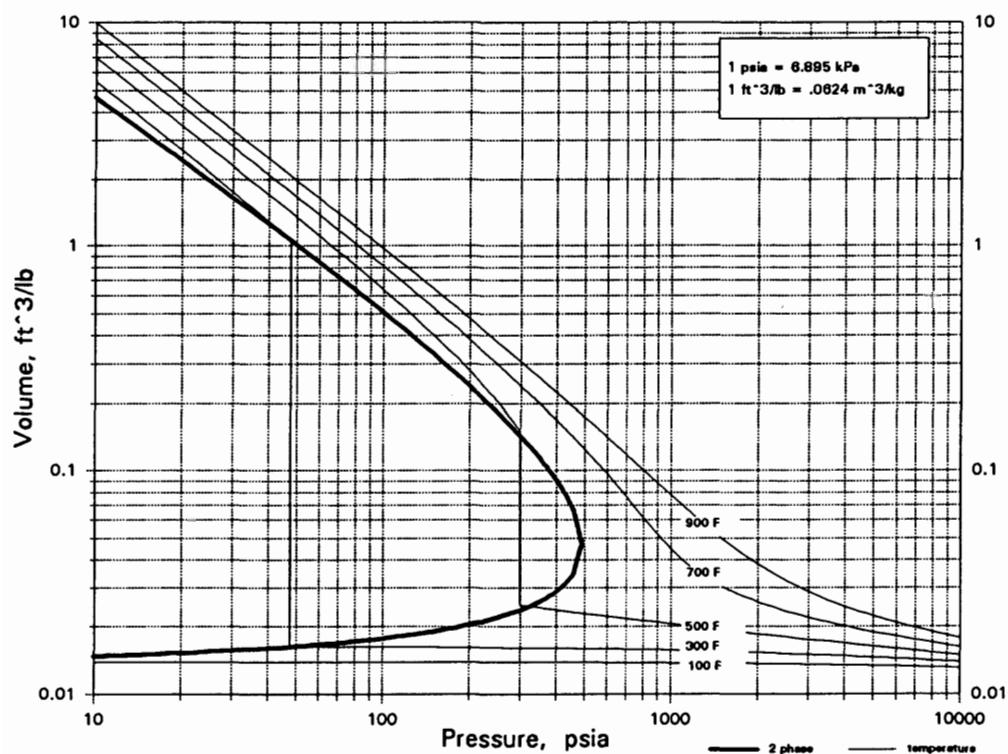


C7H5Cl3
BENZOTRICHLORIDE



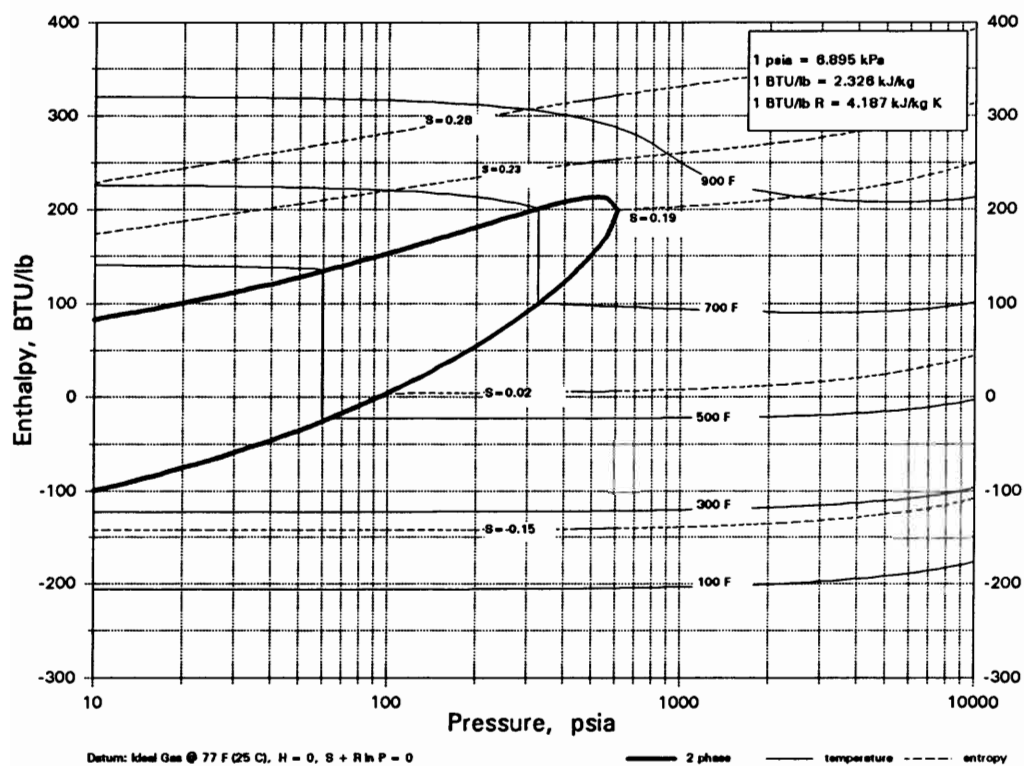
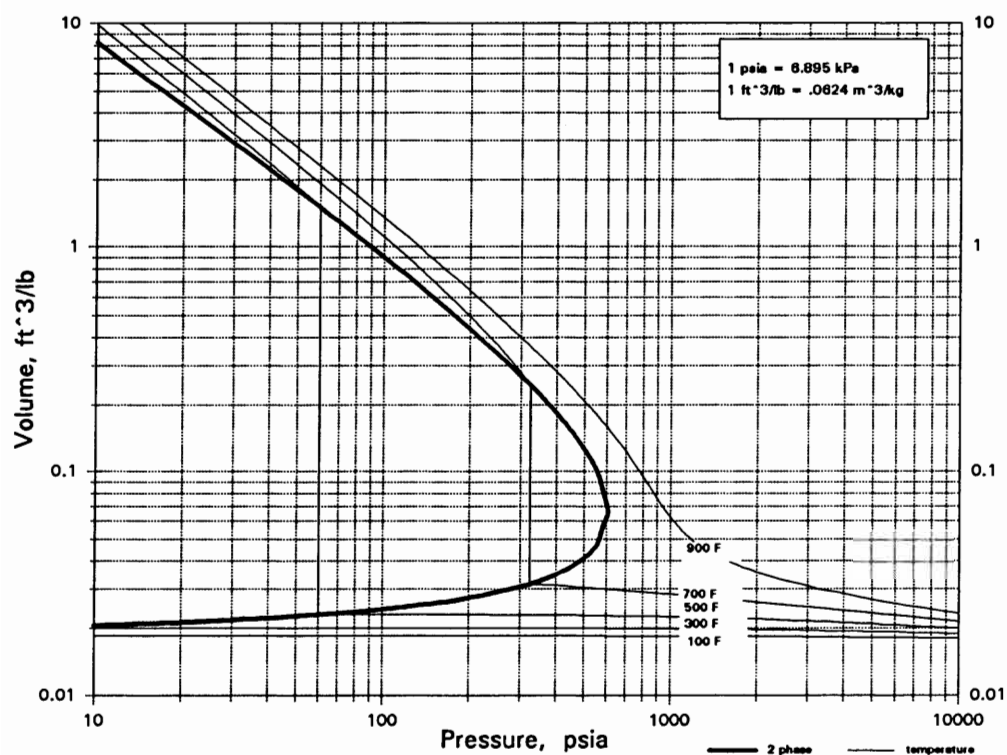
C7H5F3

BENZOTRIFLUORIDE



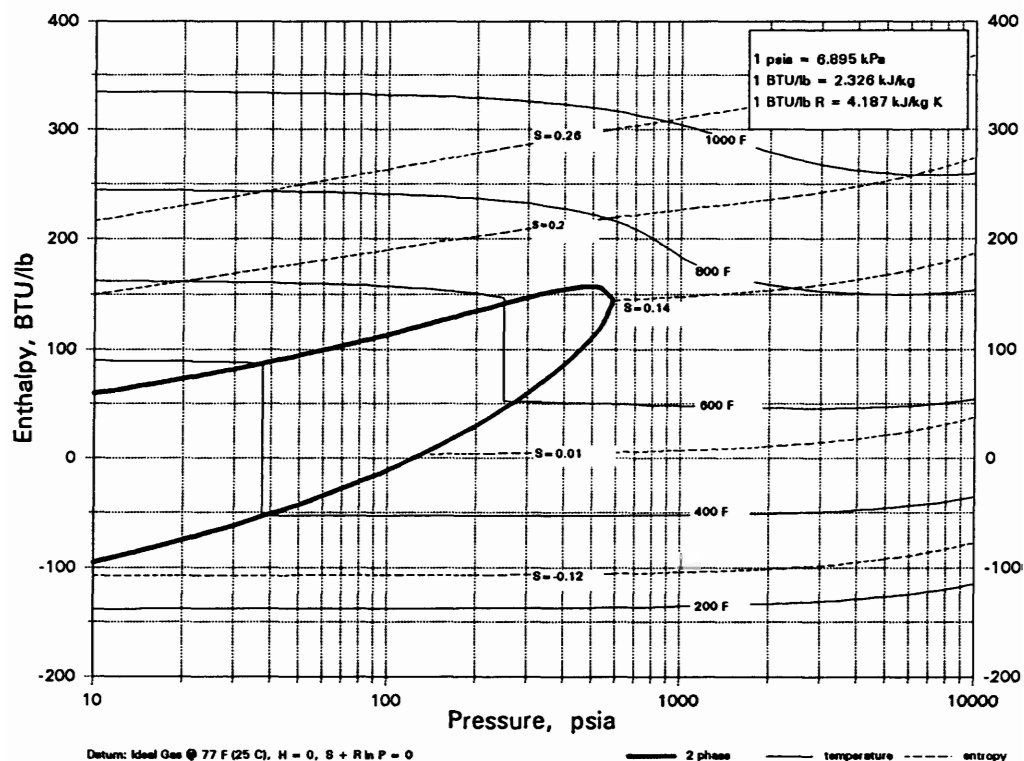
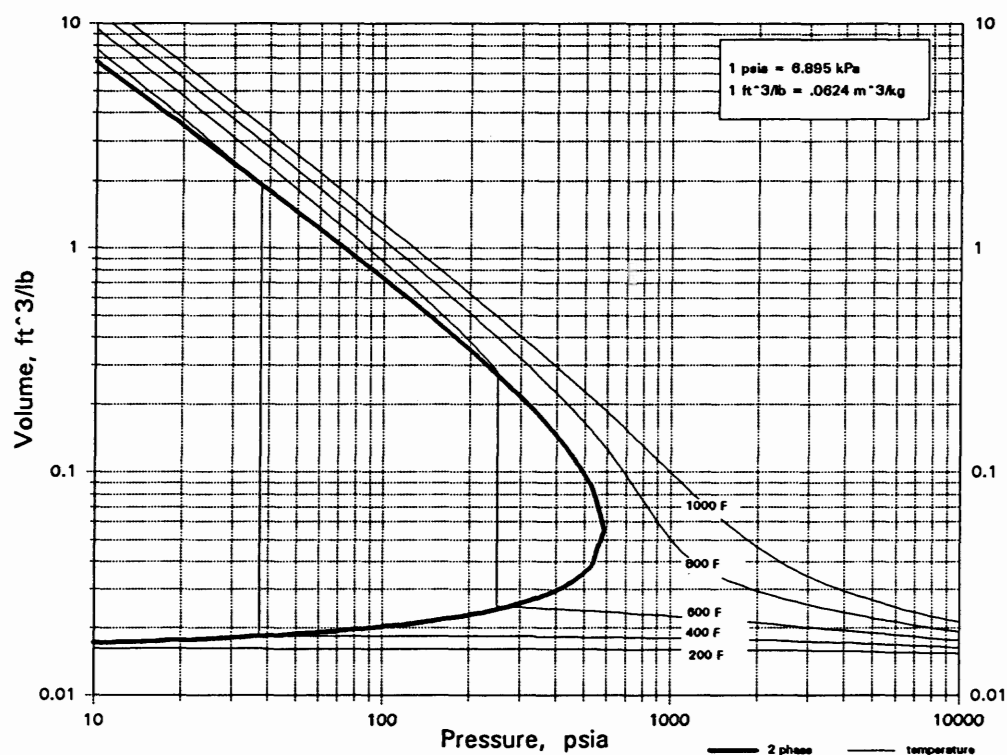
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BENZONITRILE

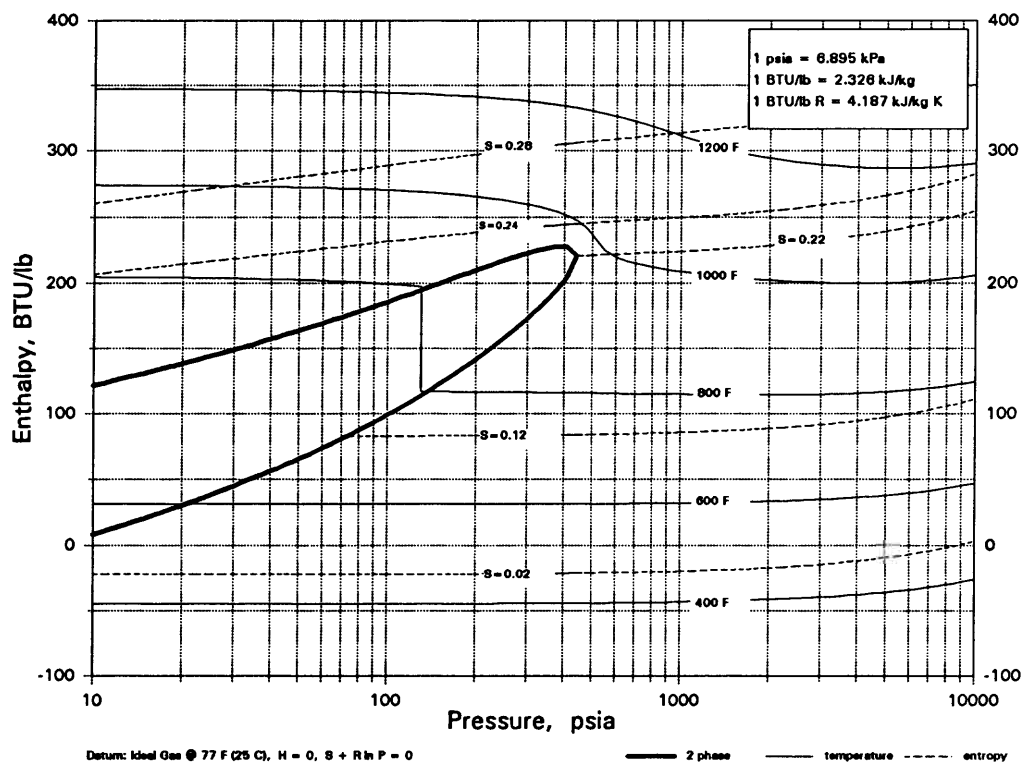
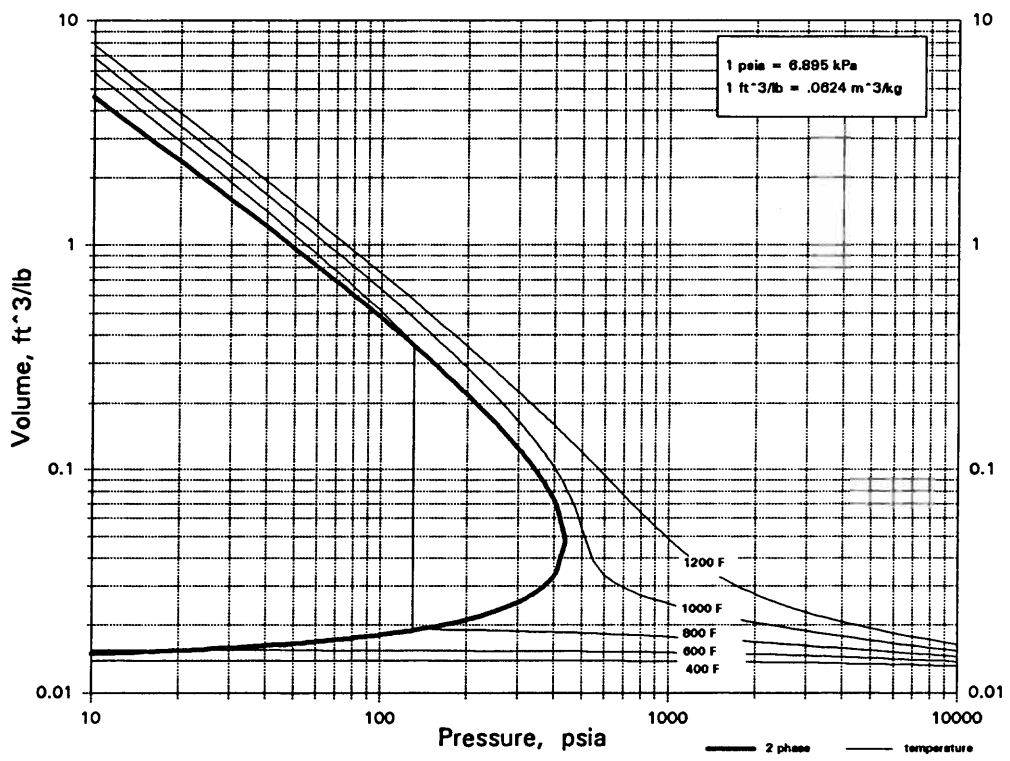


C7H5NO

PHENYL ISOCYANATE

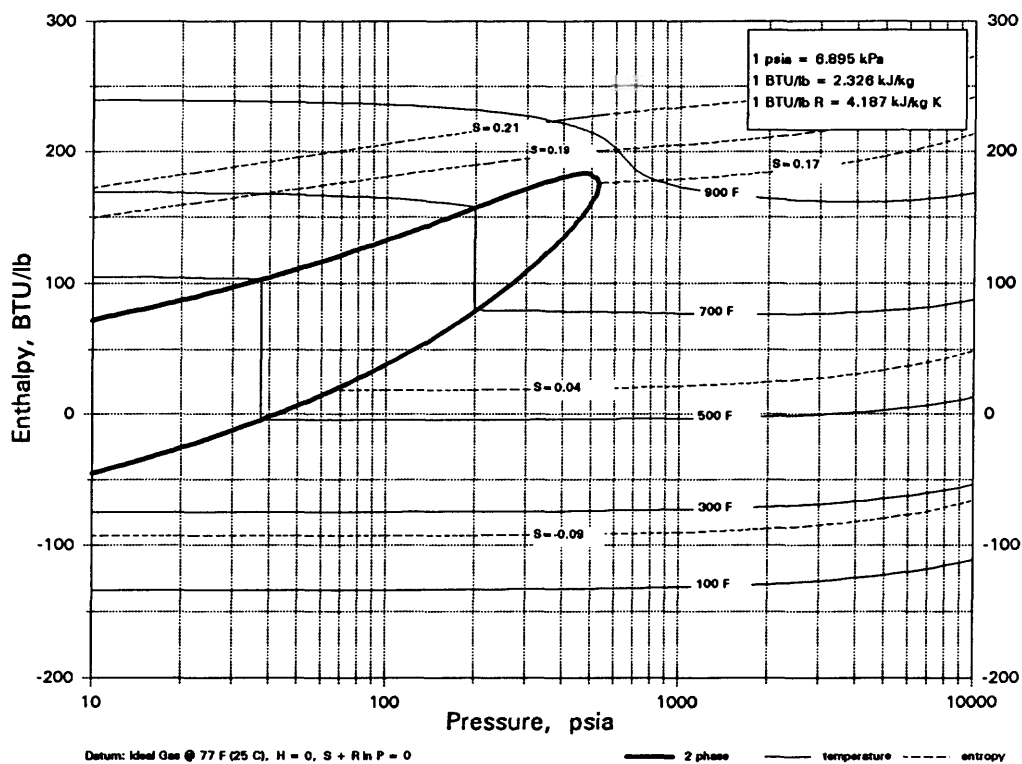
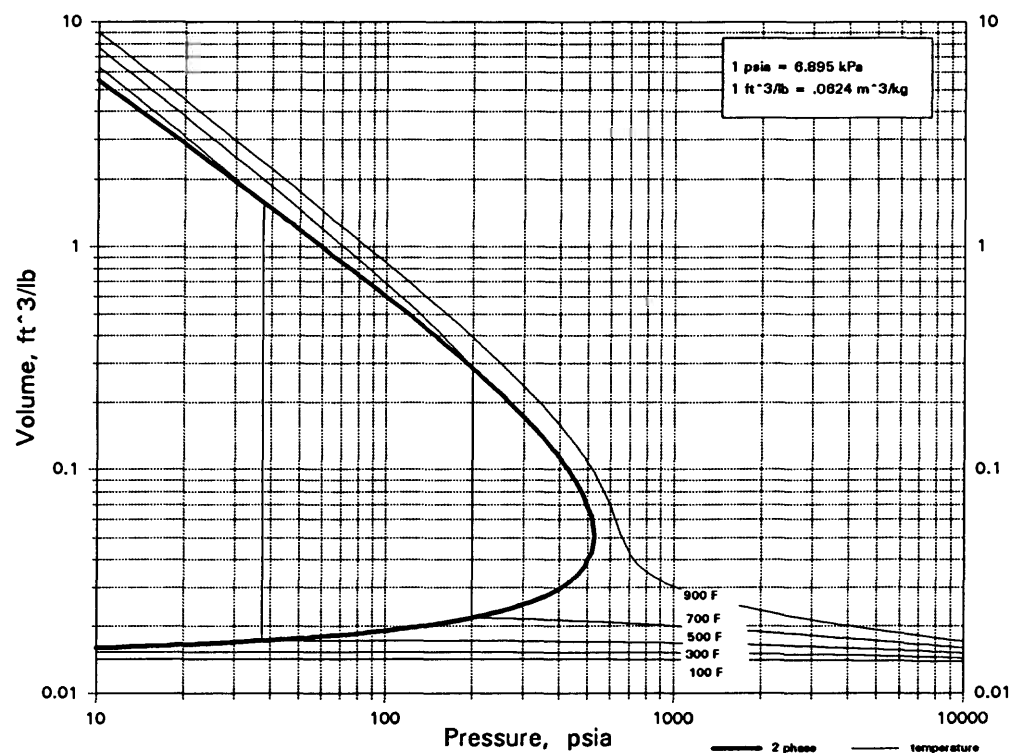


C7H5N3O6 2-4-6-TRINITROTOLUENE



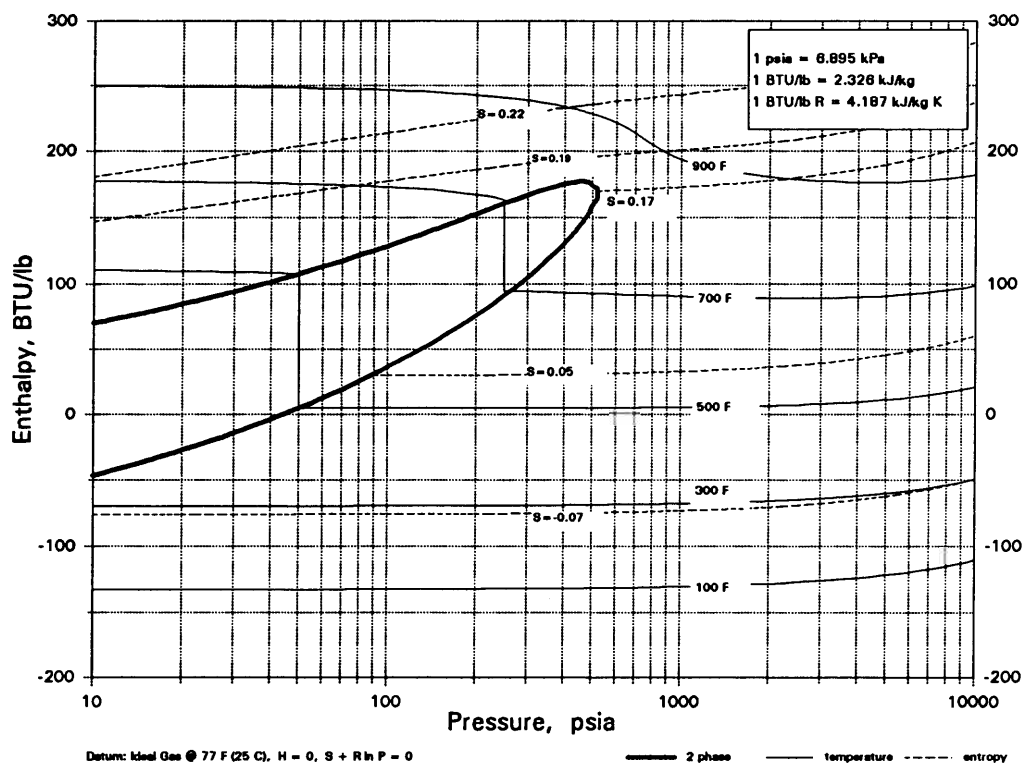
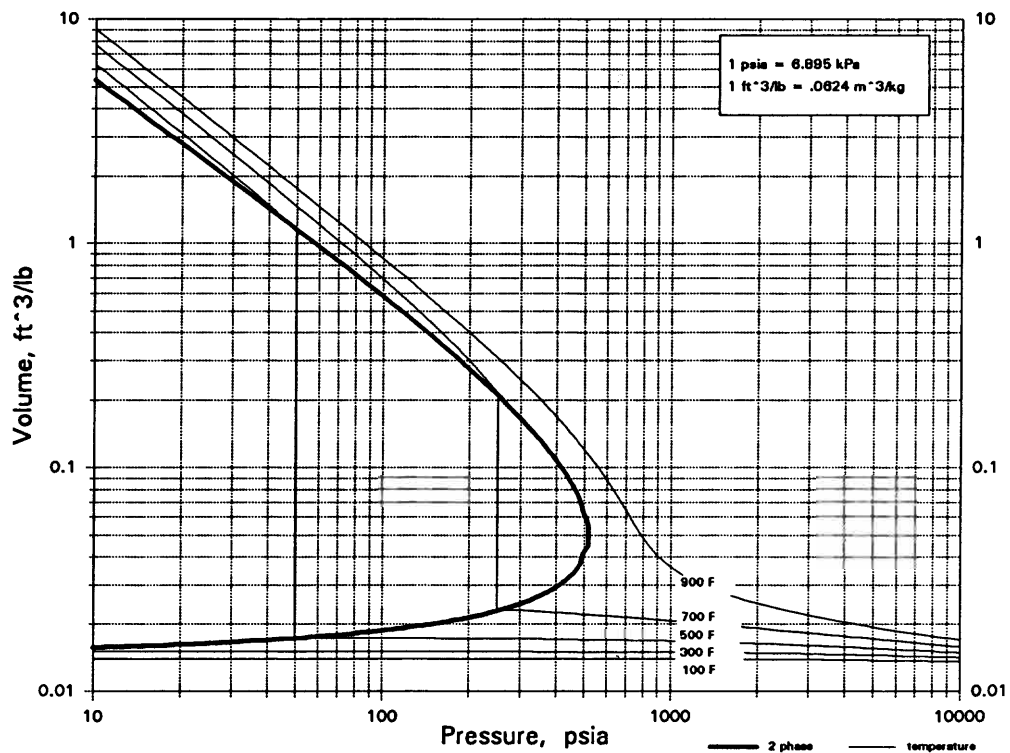
C7H6Cl2

BENZYL DICHLORIDE

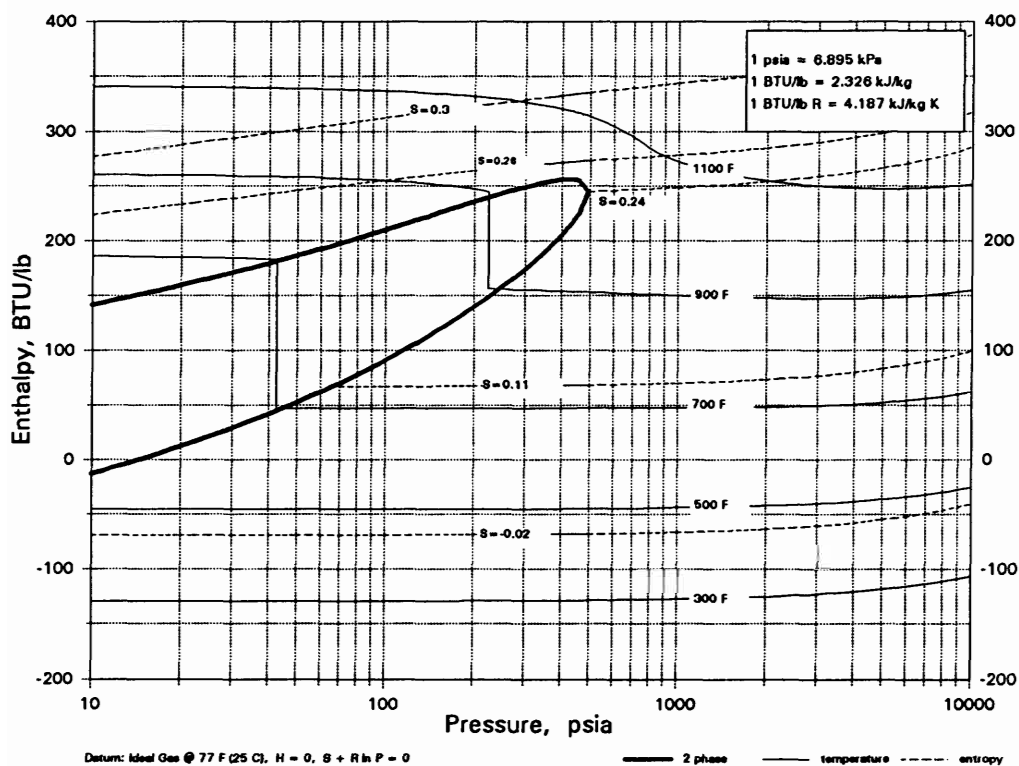
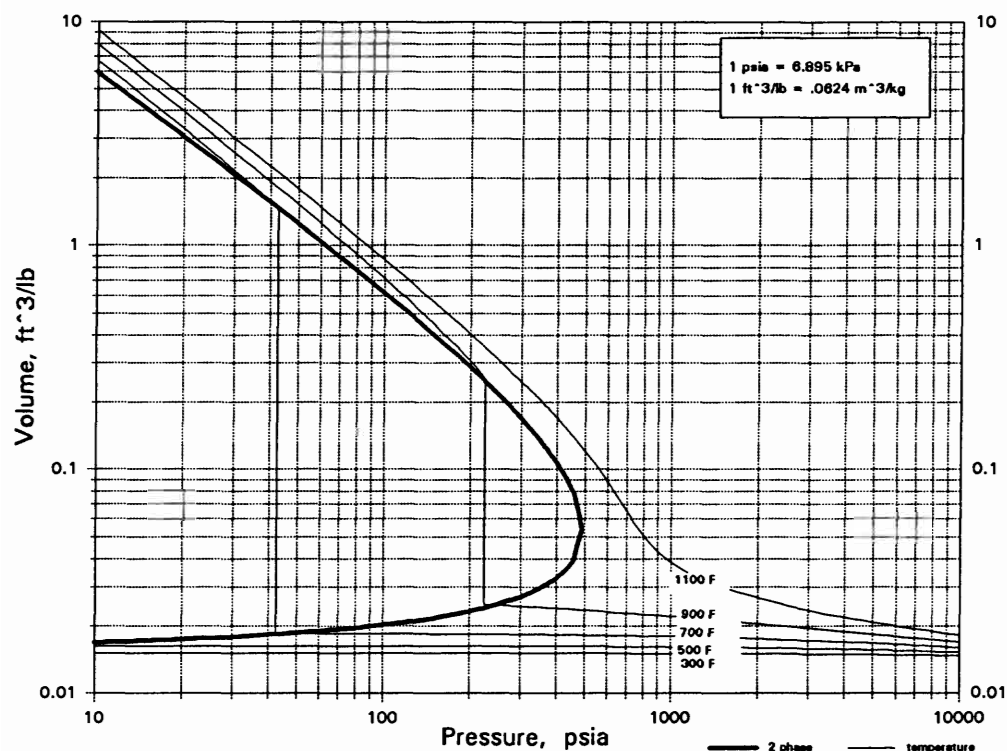


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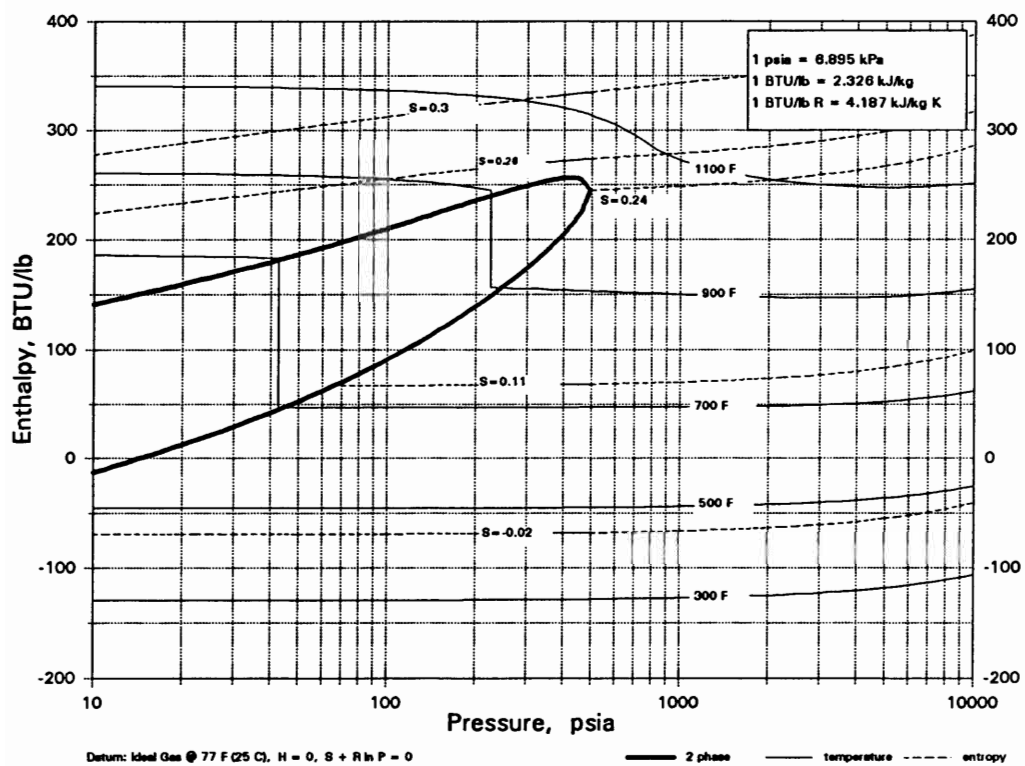
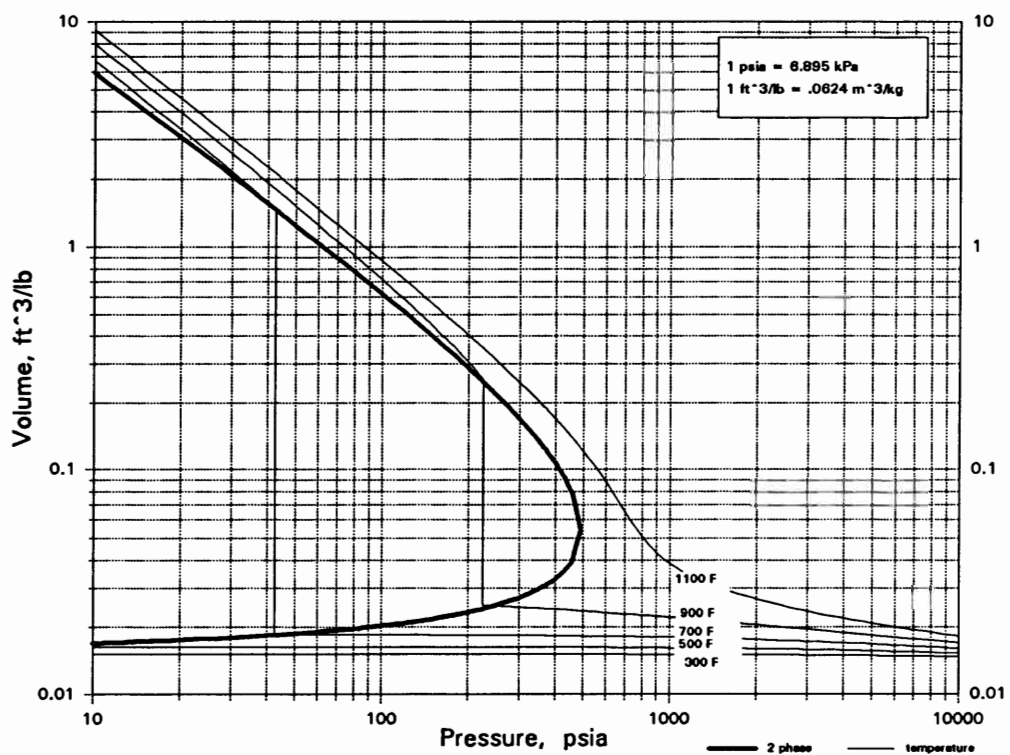
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C7H6N2O4 2,4-DINITROTOLUENE

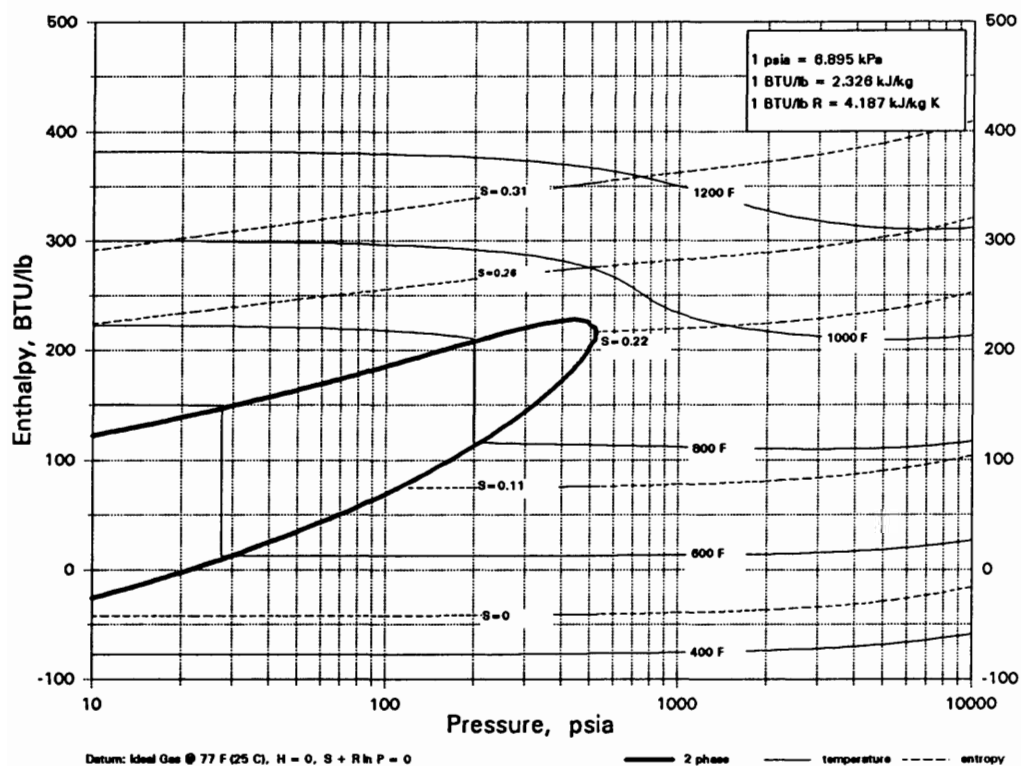
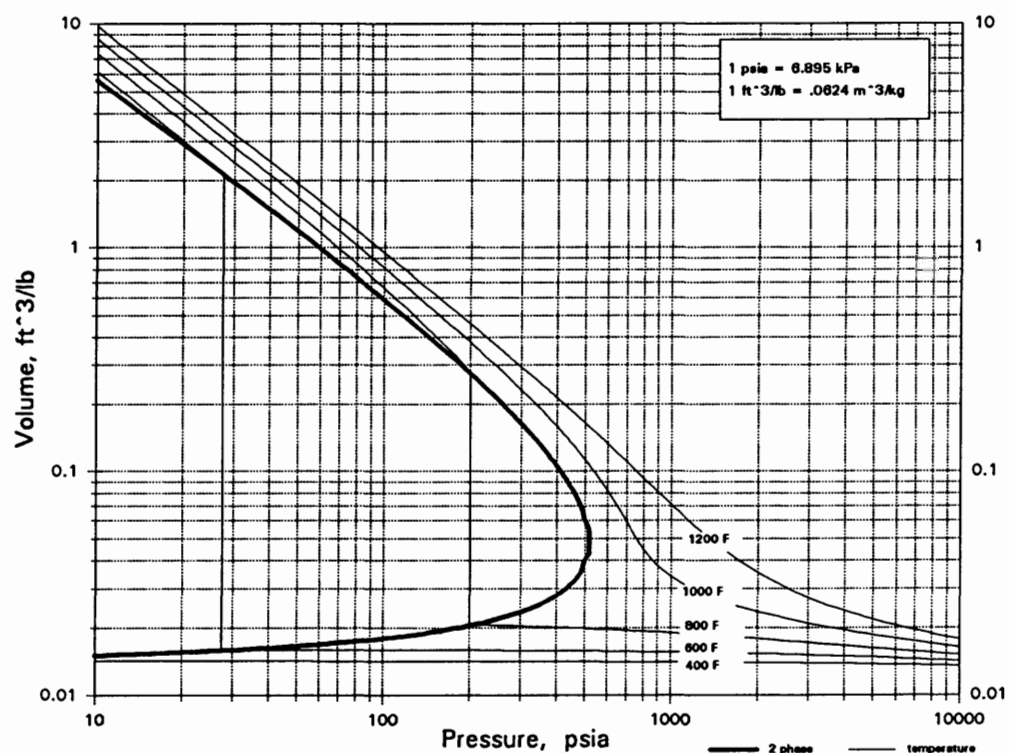


C7H6N2O4
2-5-DINITROTOLUENE



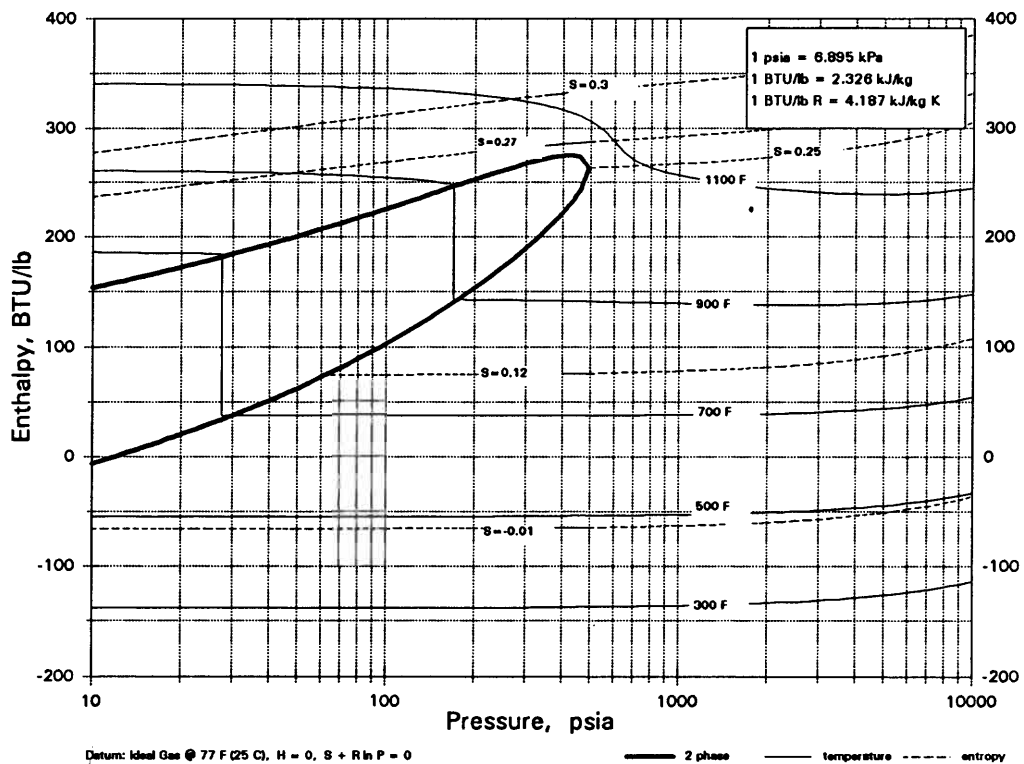
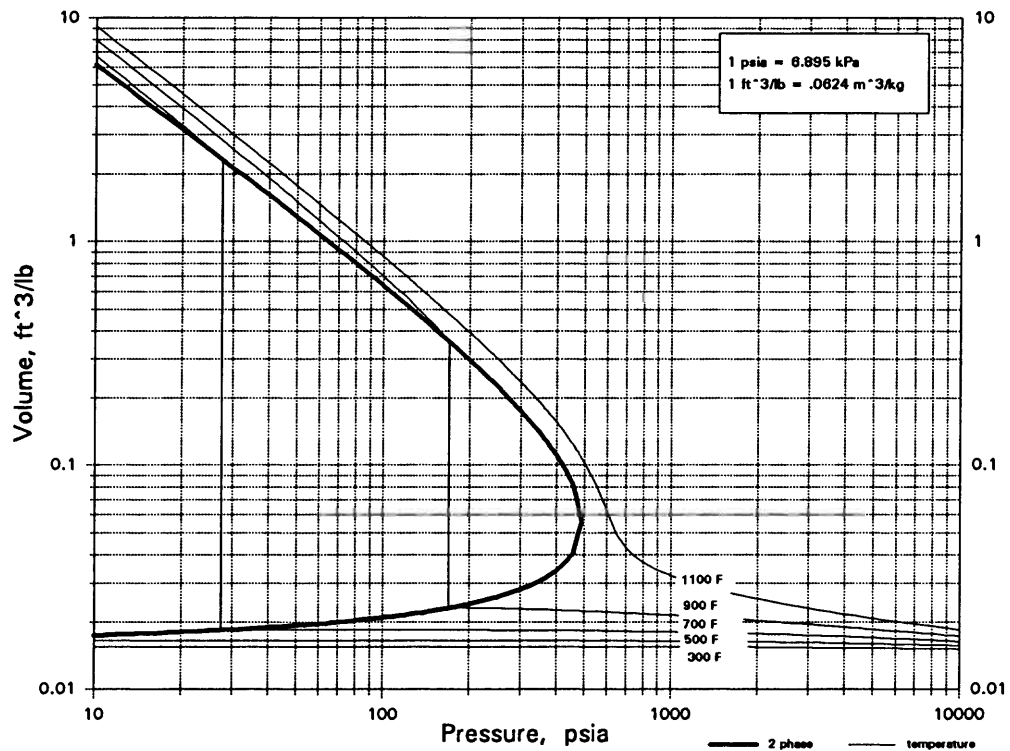
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2-6-DINITROTOLUENE



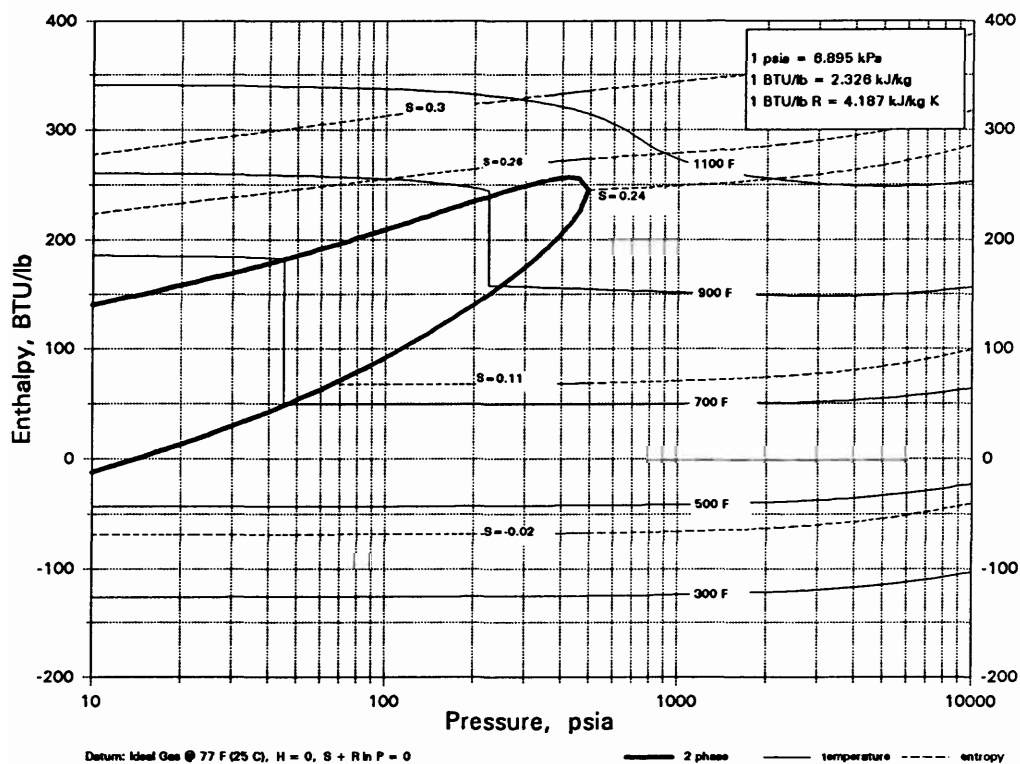
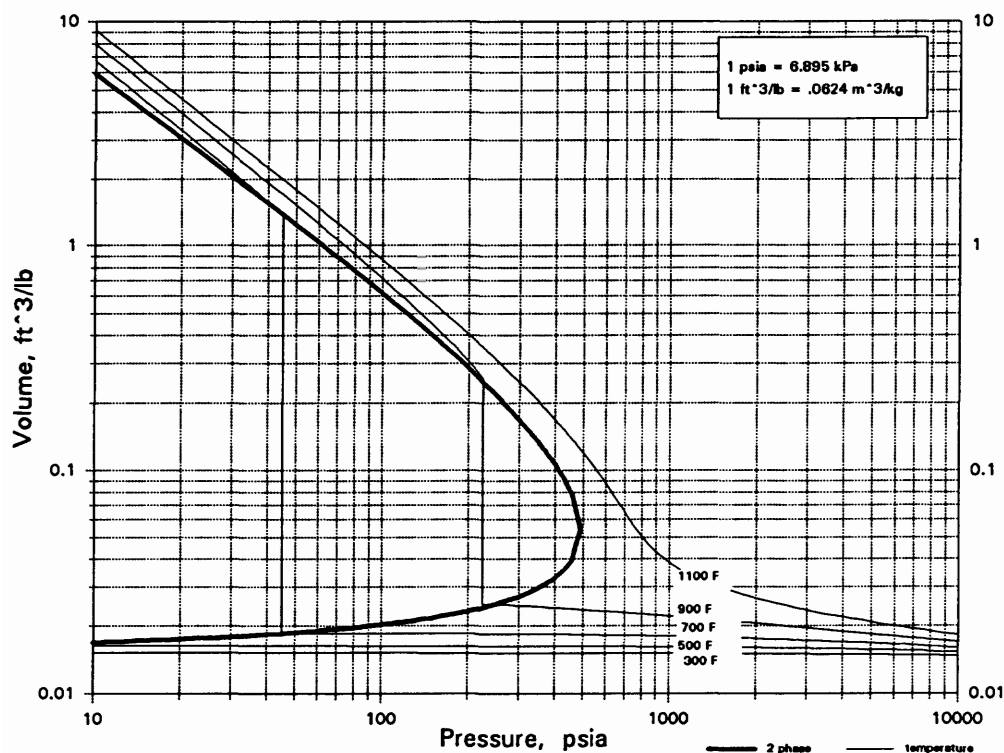
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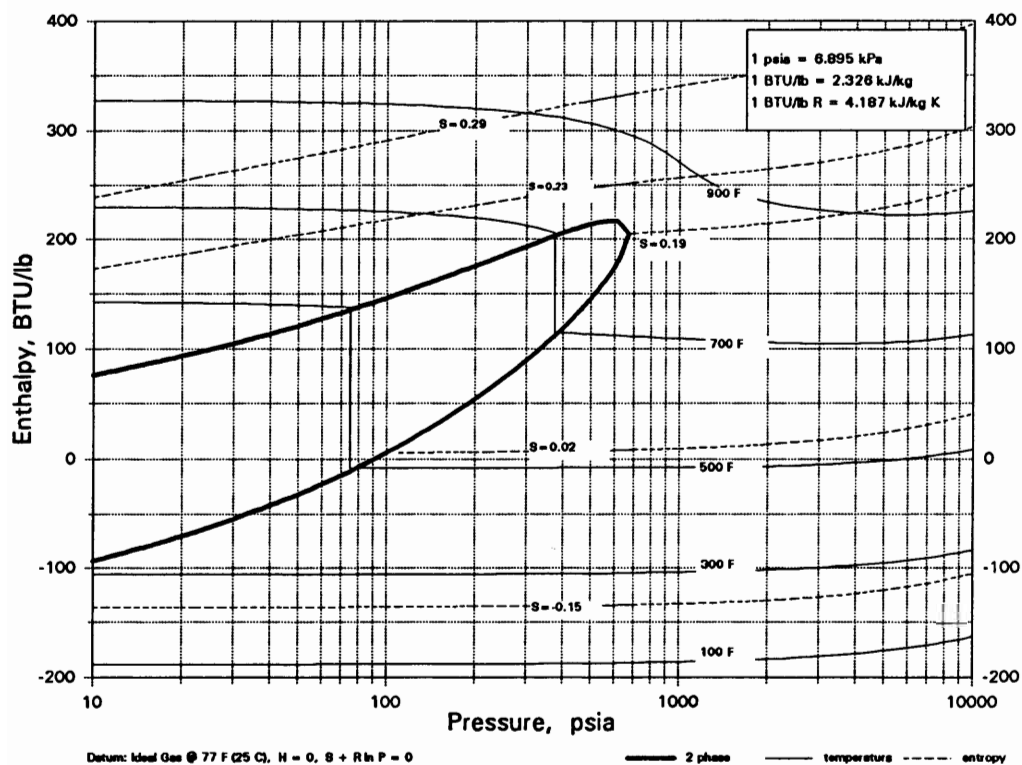
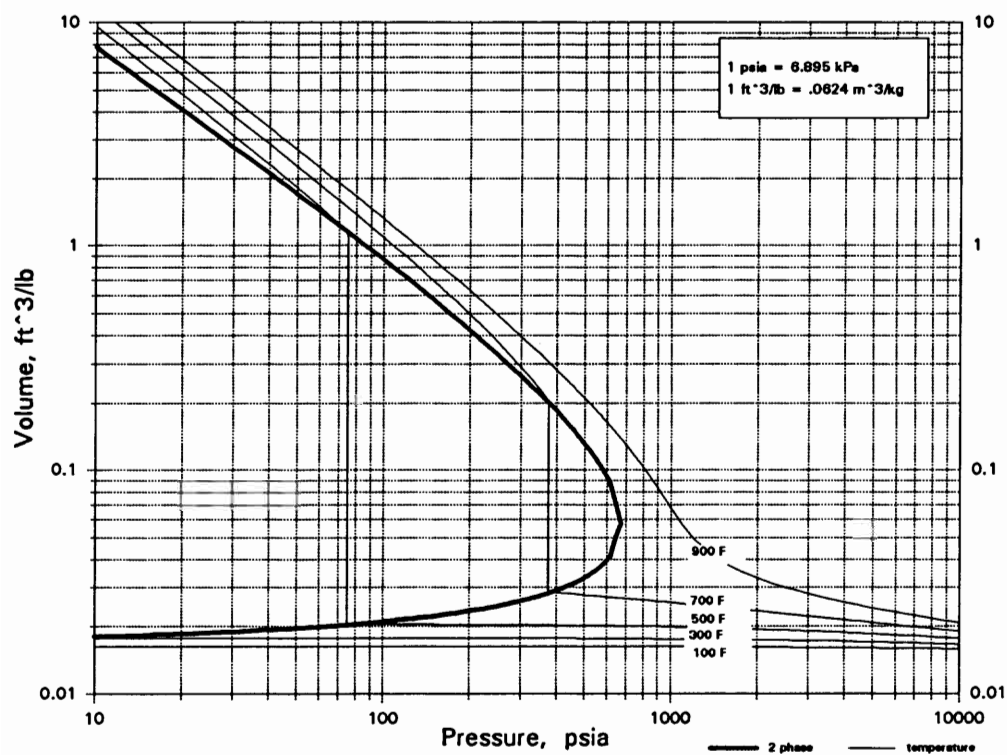
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3-5-DINITROTOLUENE



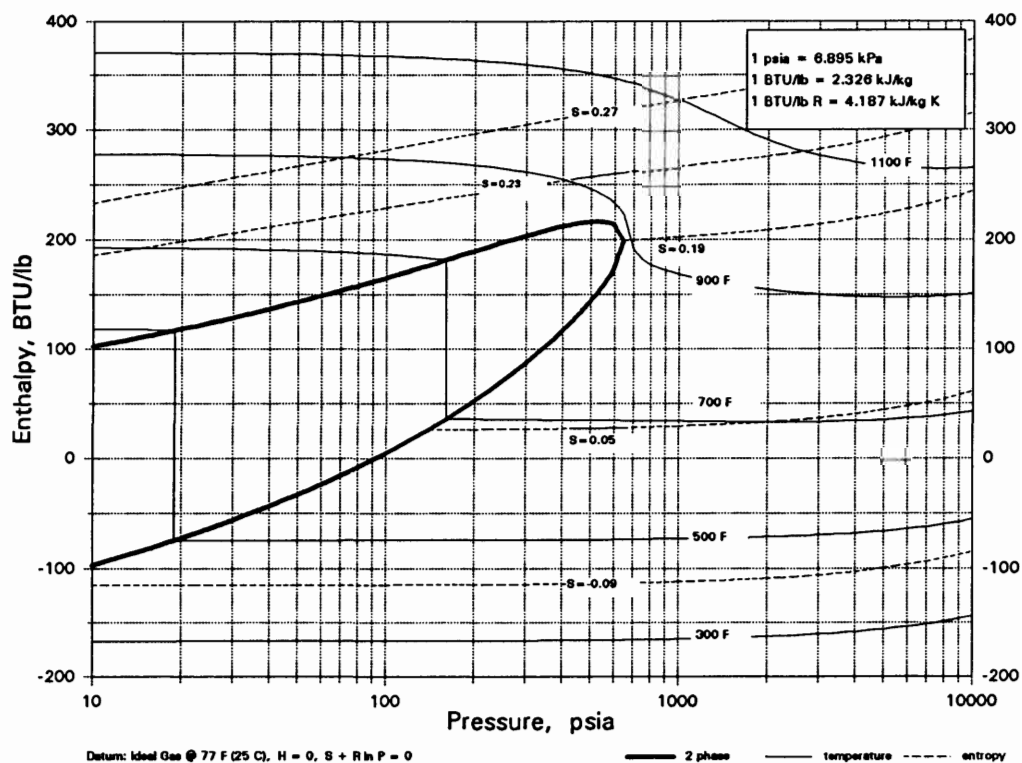
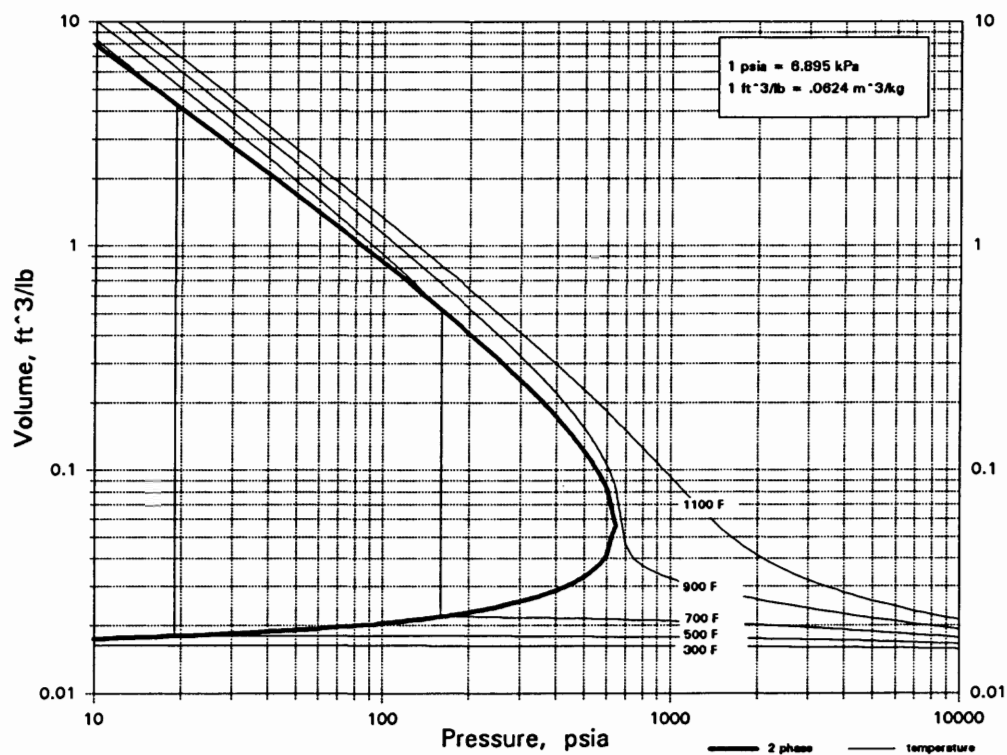
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BENZALDEHYDE



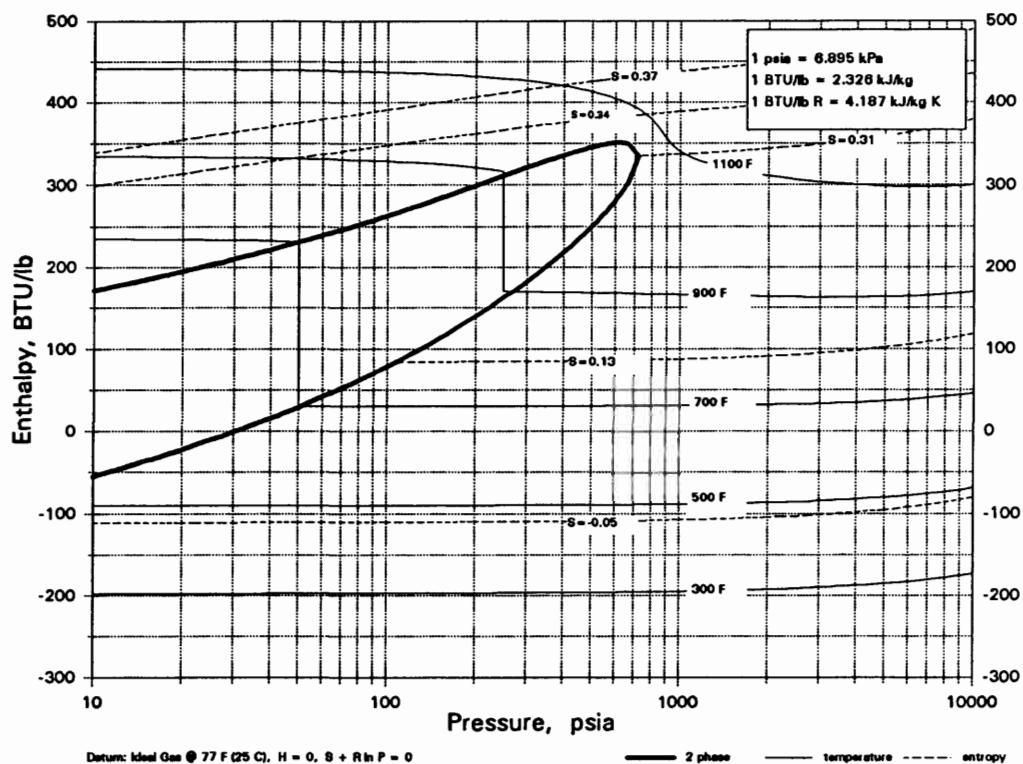
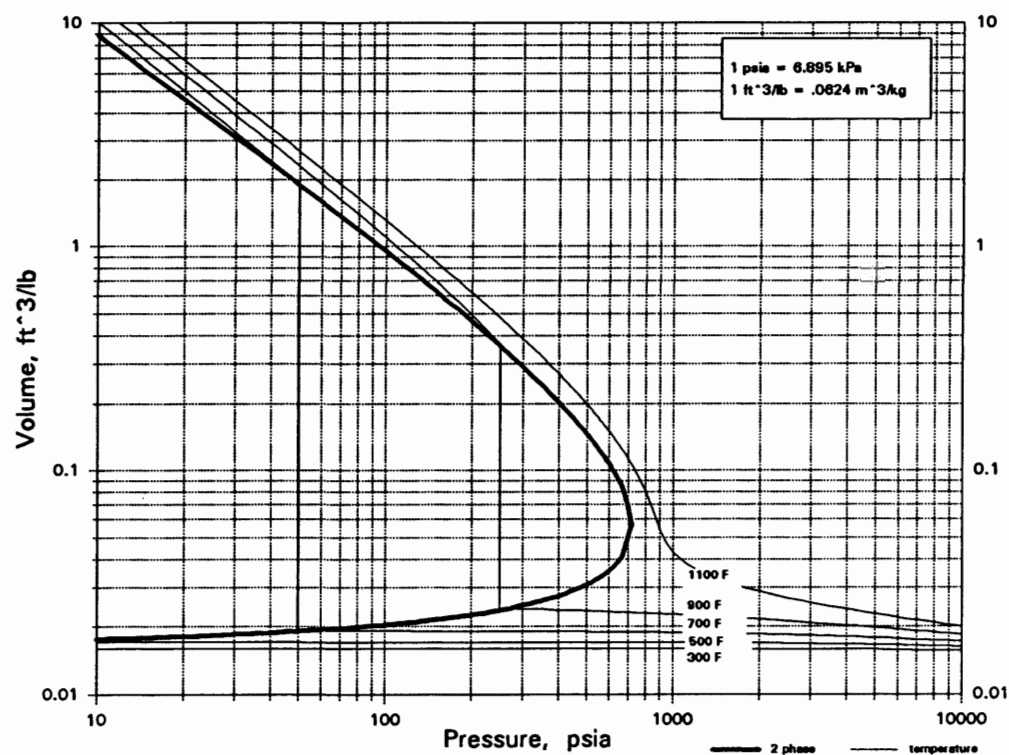
C7H6O2

BENZOIC ACID



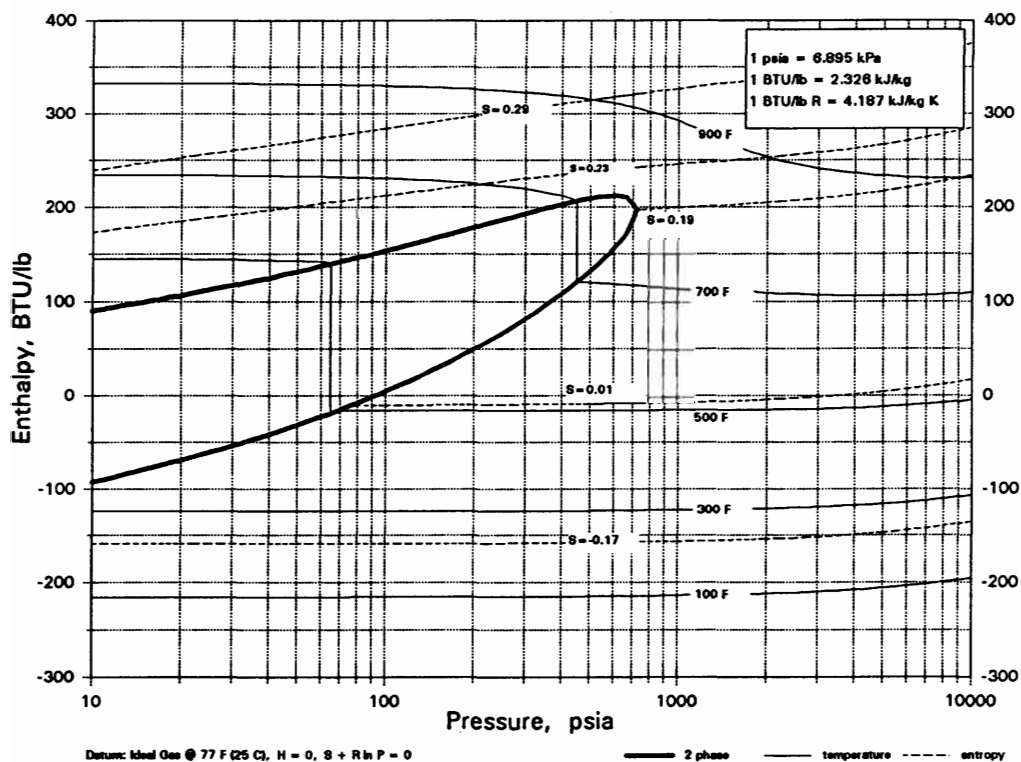
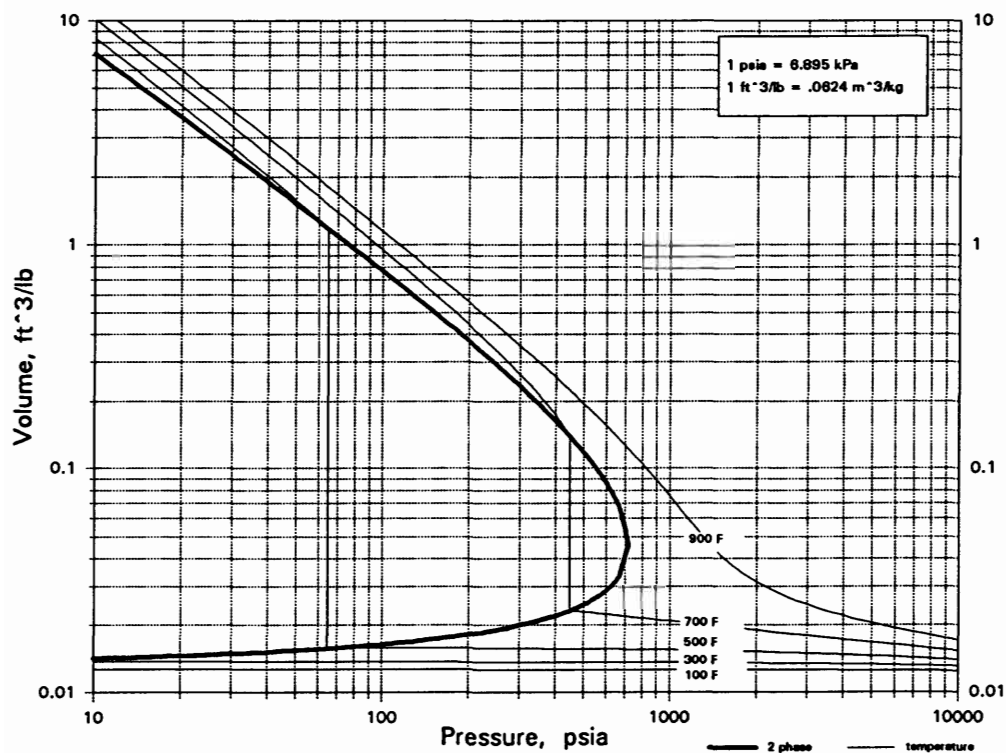
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p-HYDROXYBENZALDEHYDE



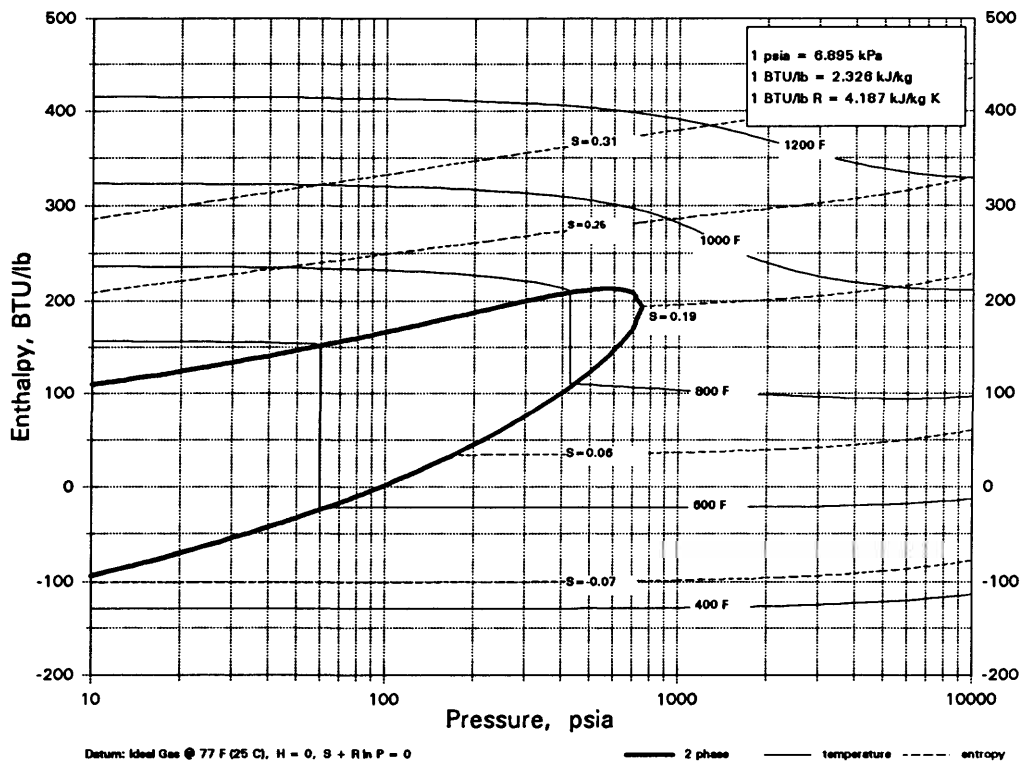
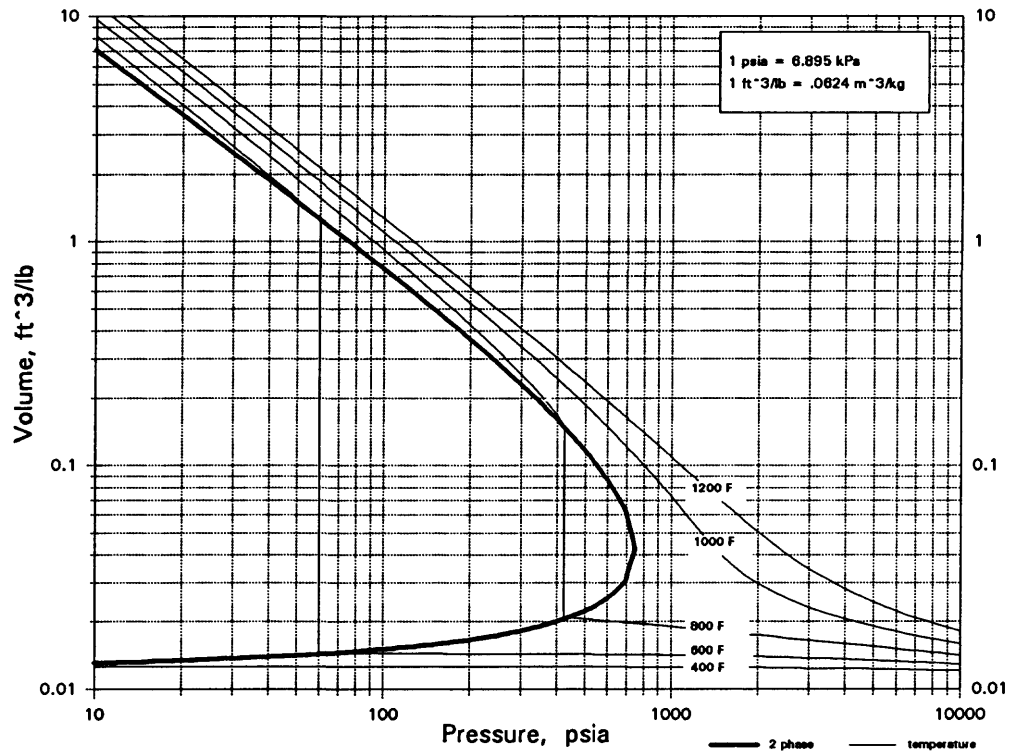
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SALICYLALDEHYDE



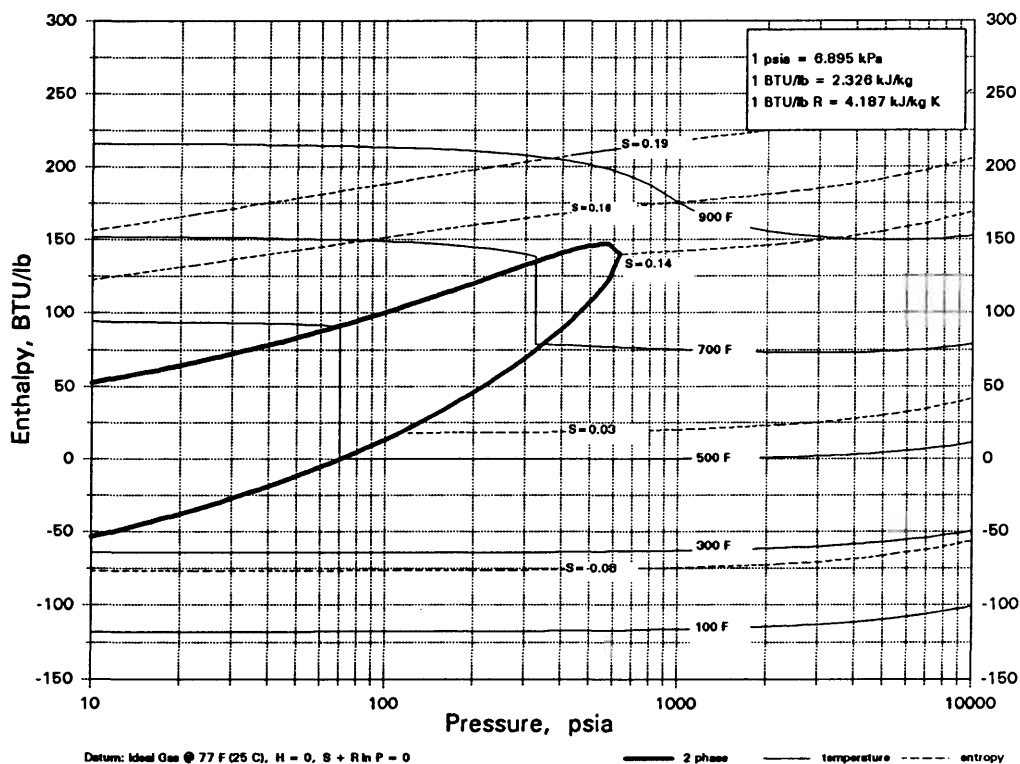
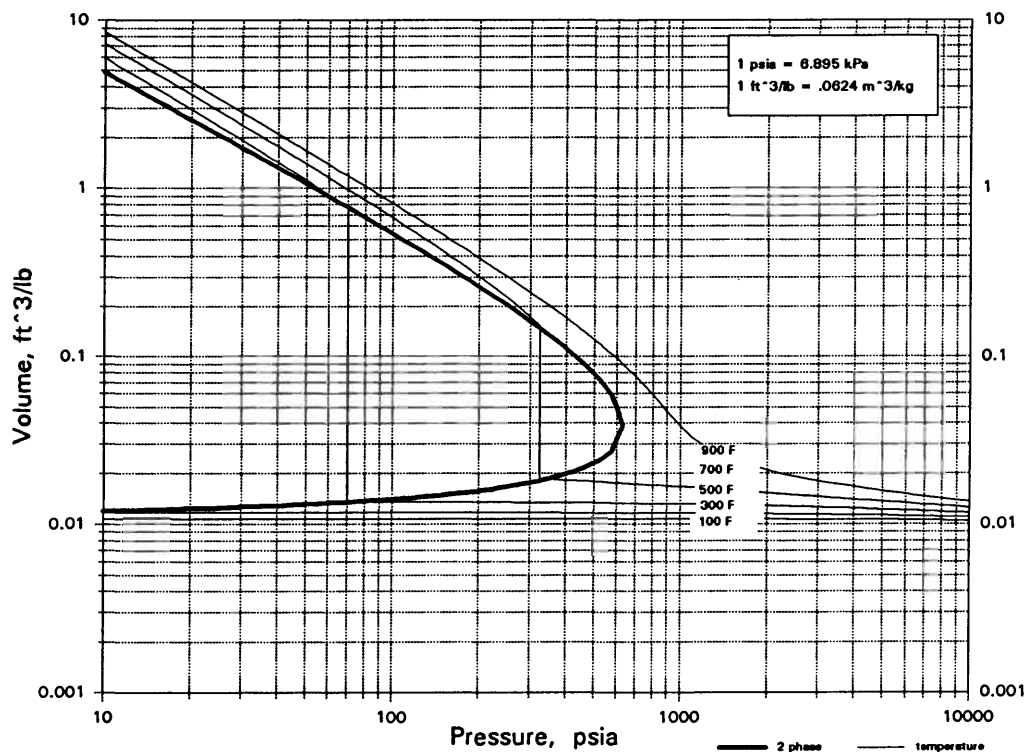
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SALICYLIC ACID



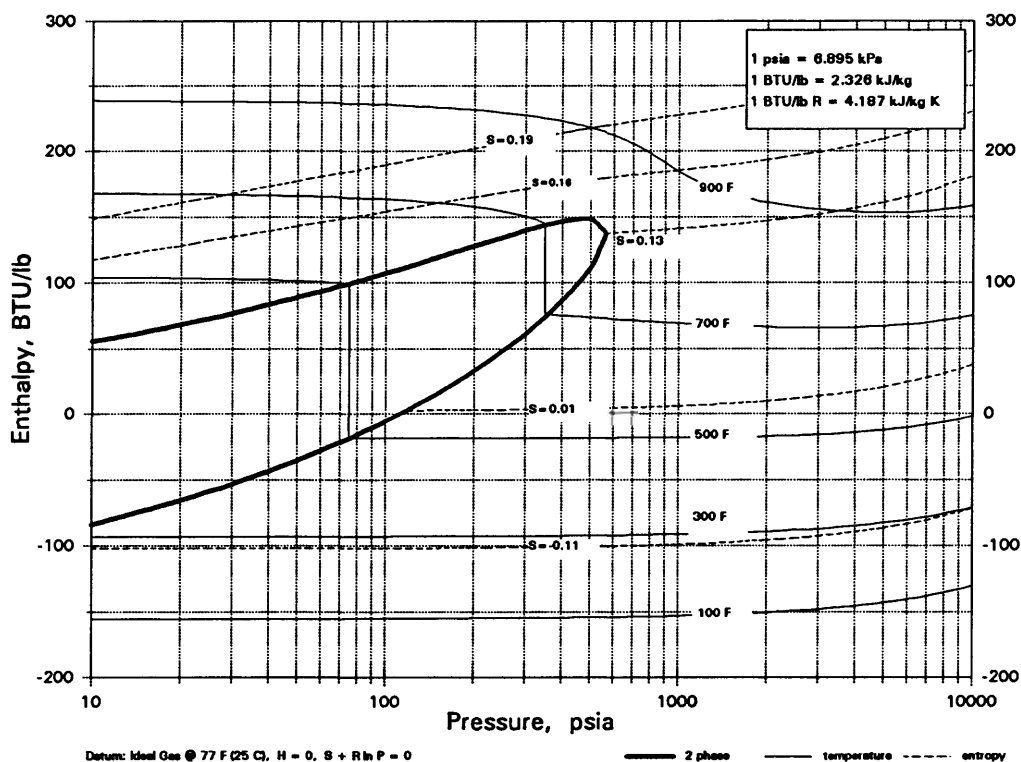
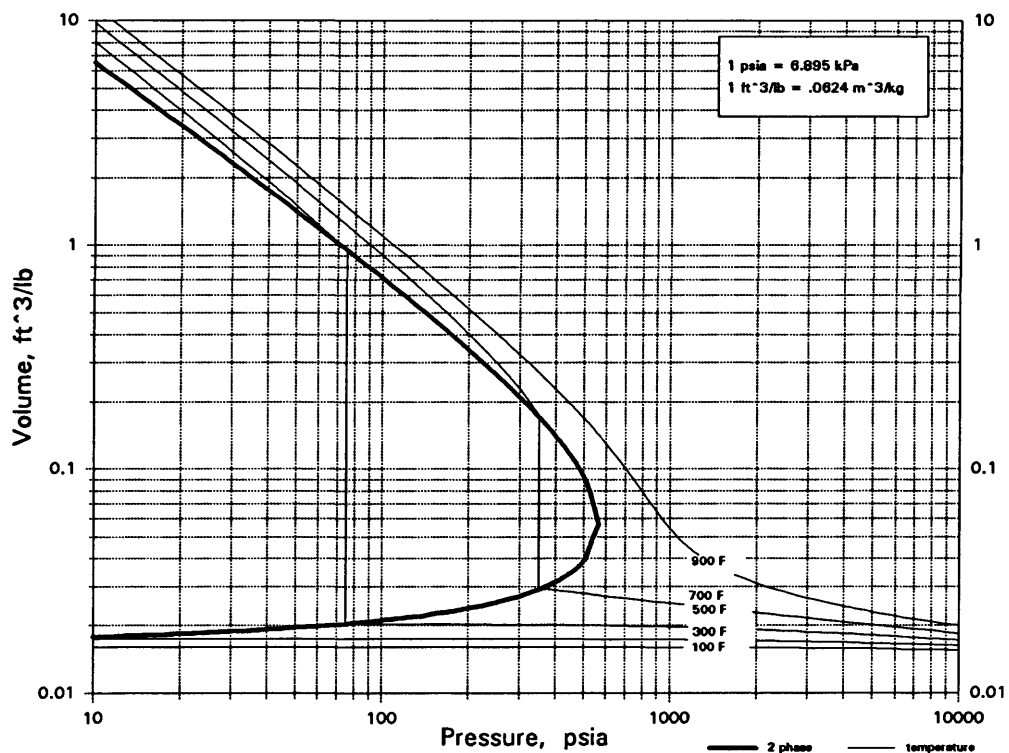
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p-BROMOTOLUENE



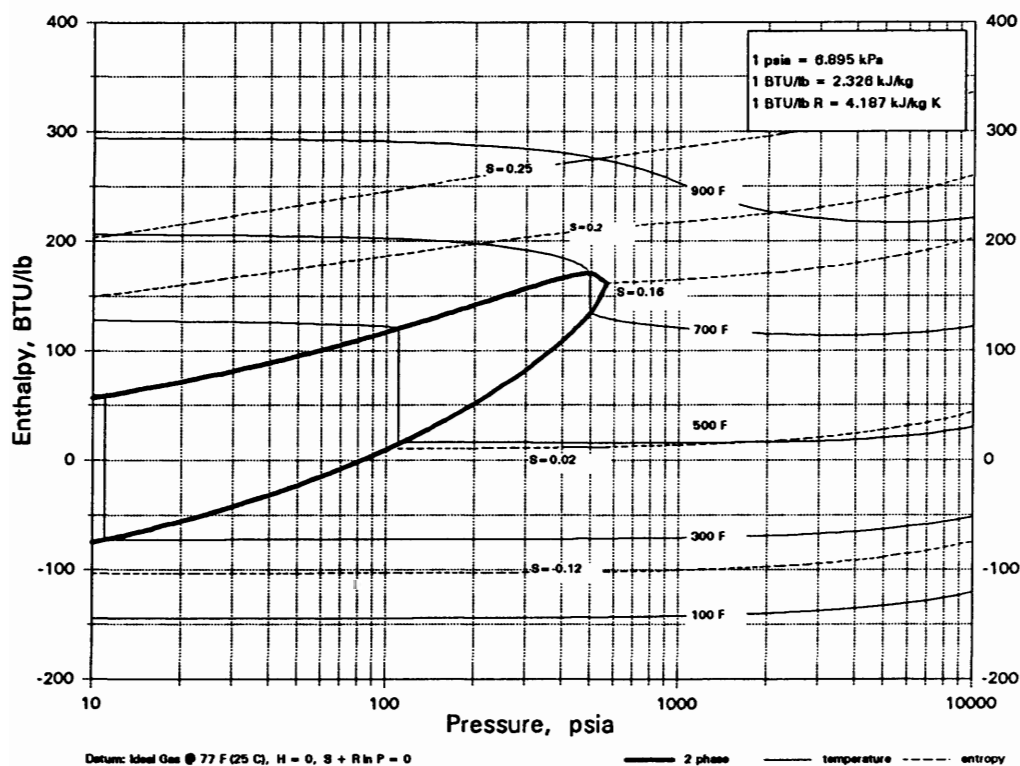
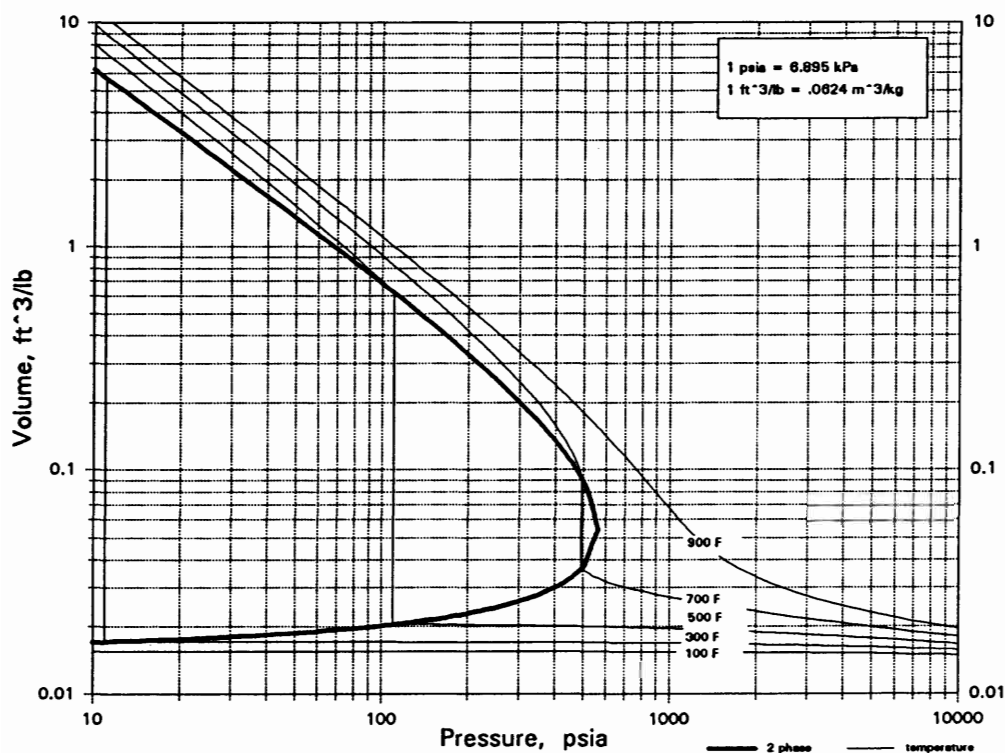
C7H7Cl

BENZYL CHLORIDE



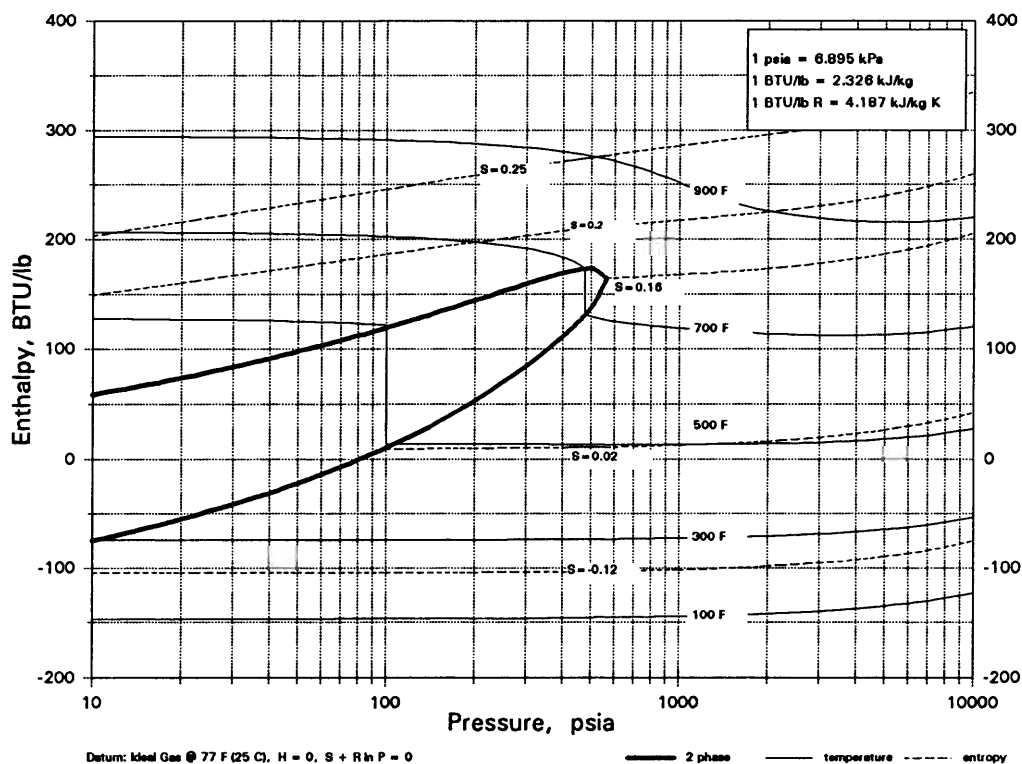
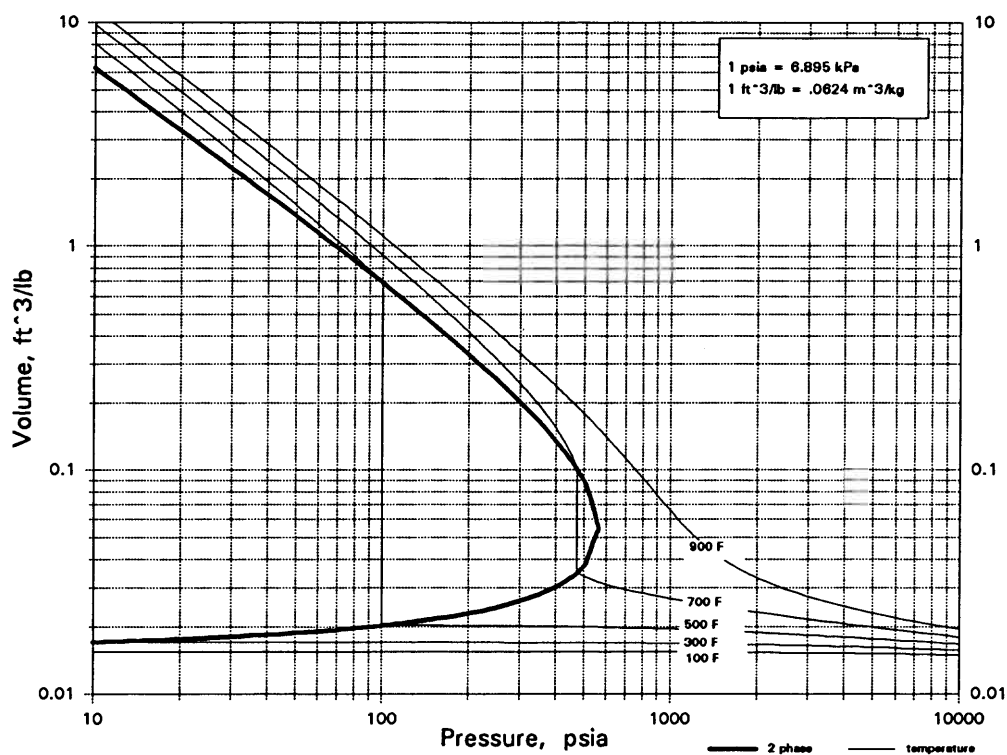
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o-CHLOROTOLUENE



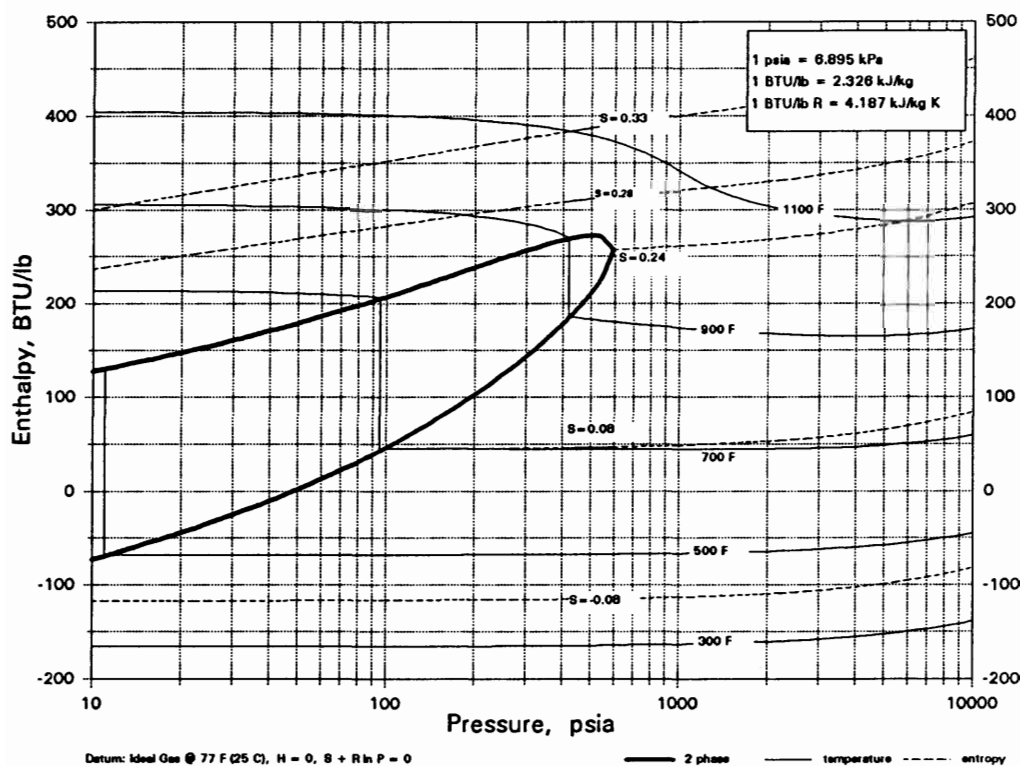
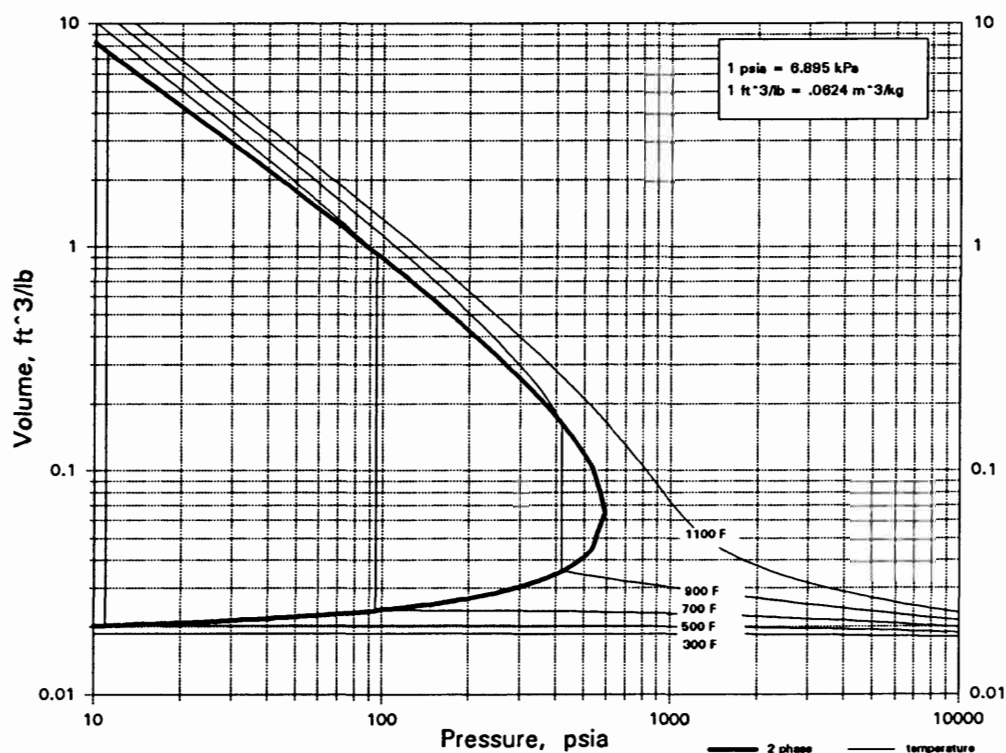
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p-CHLOROTOLUENE



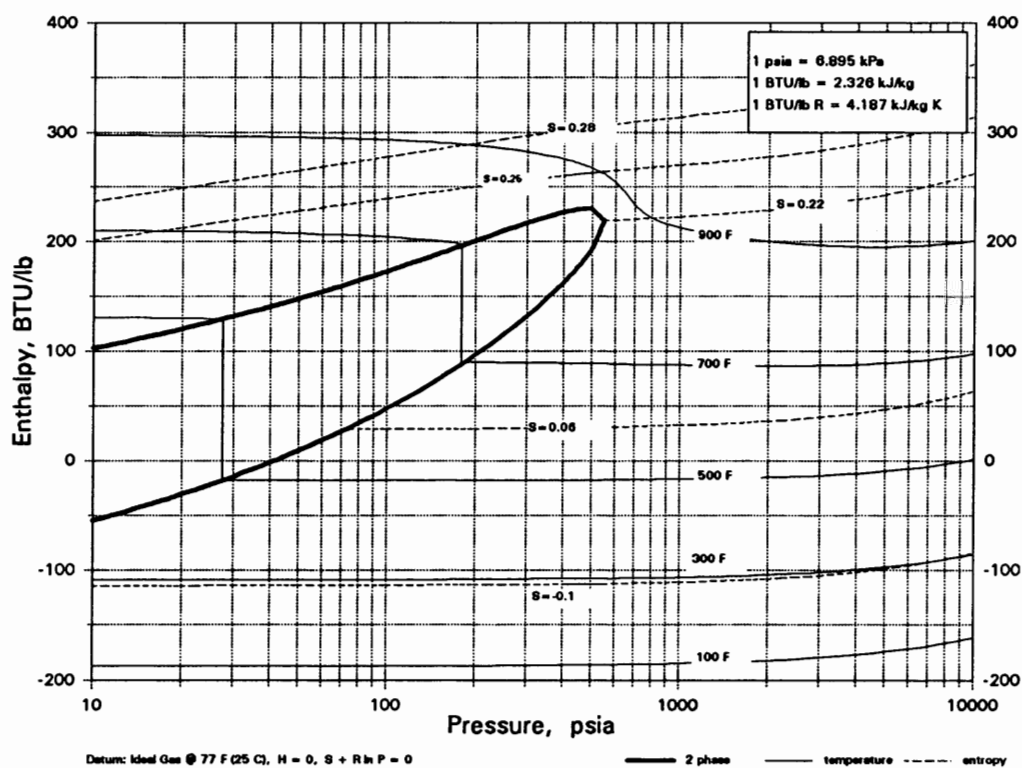
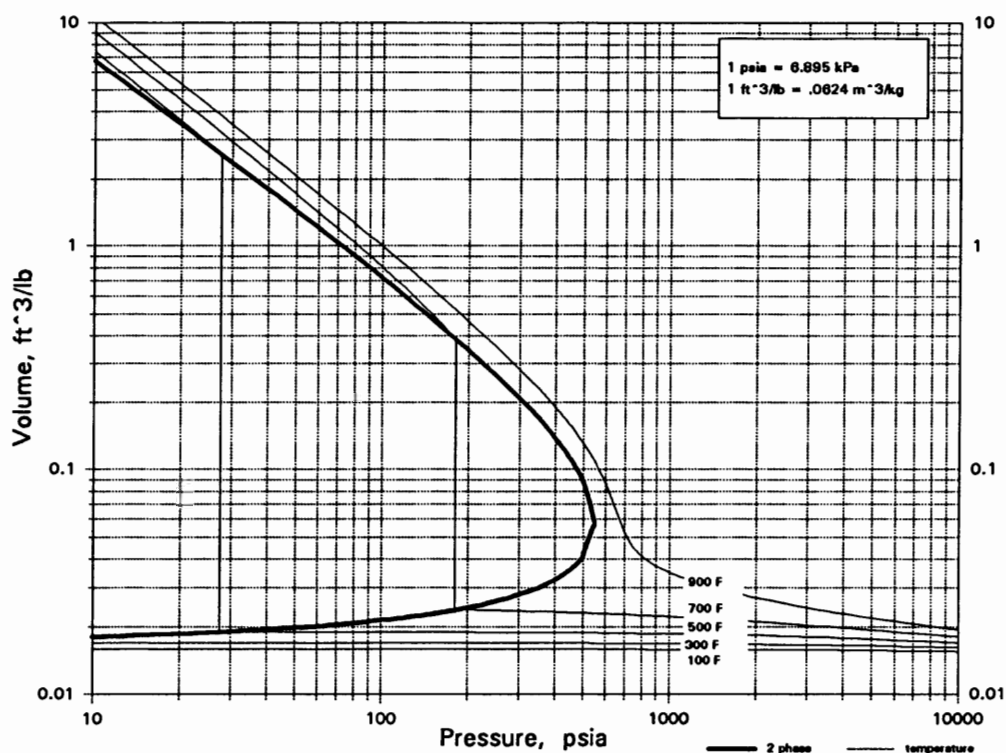
C7H7NO

FORMANILIDE

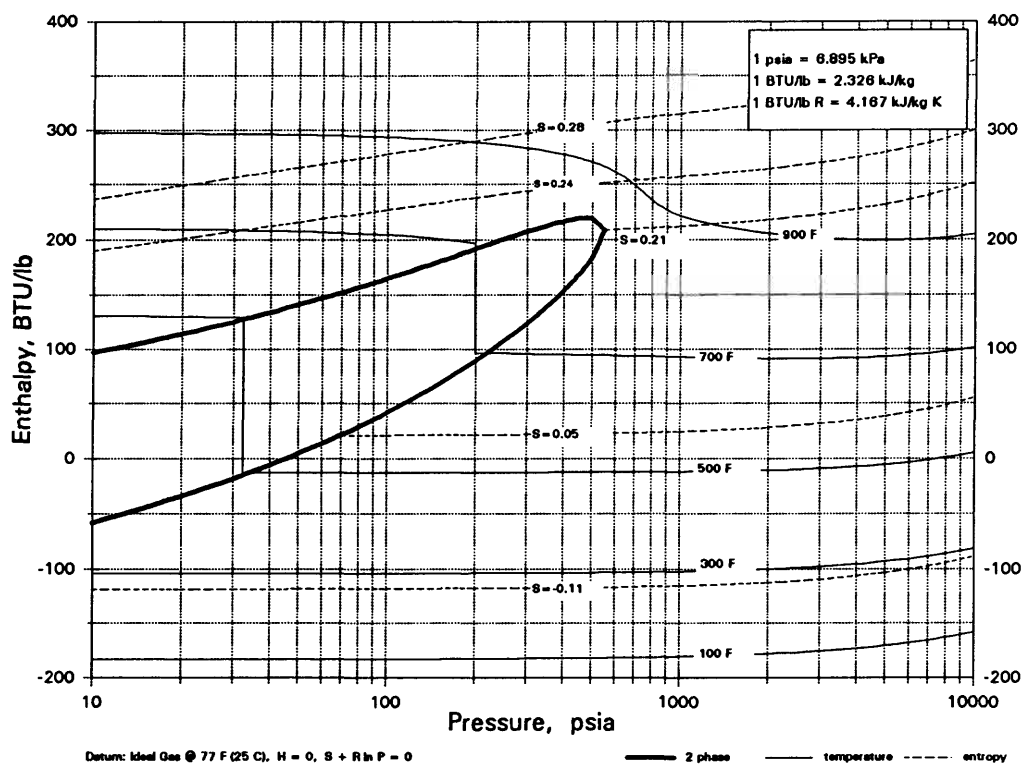
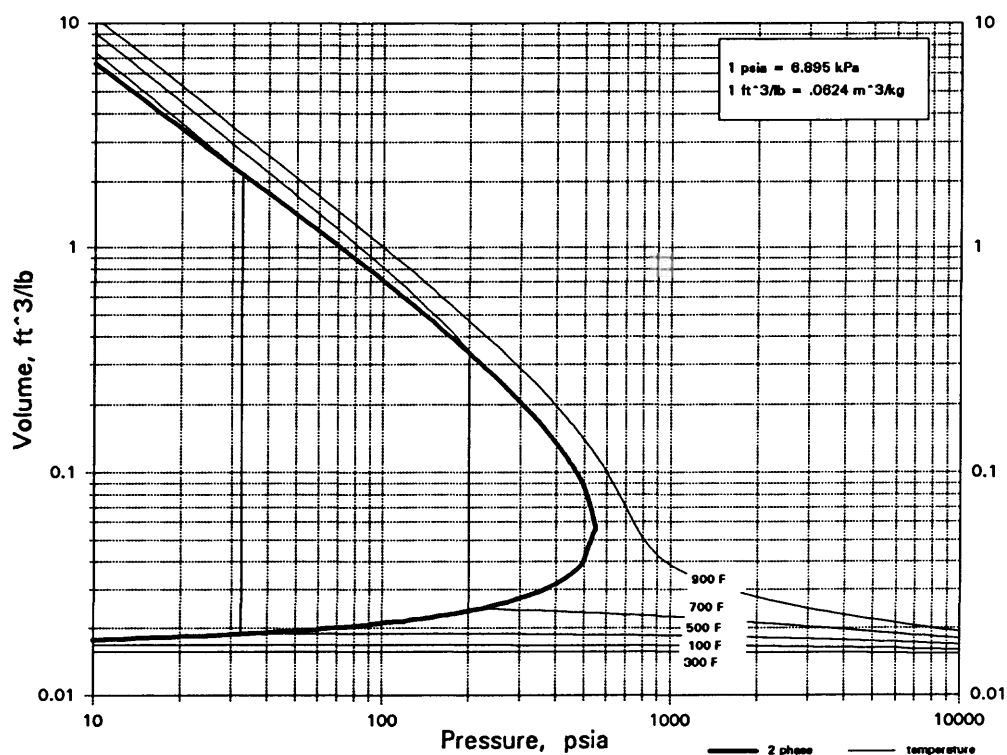


C7H7NO2

m-NITROTOLUENE

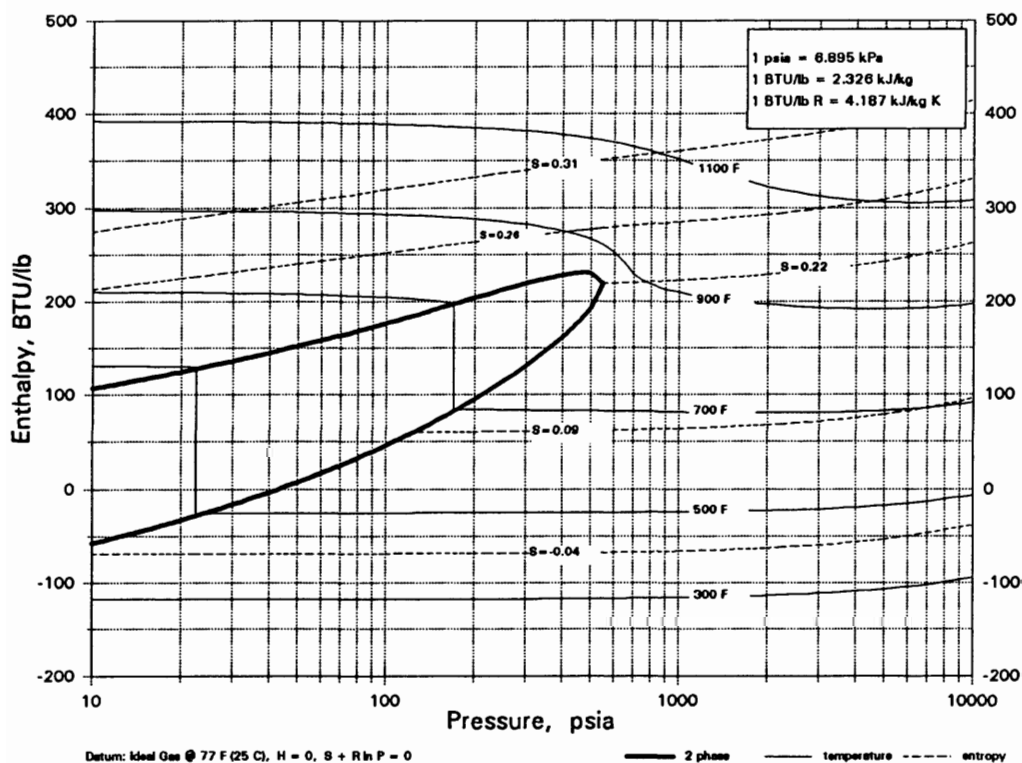
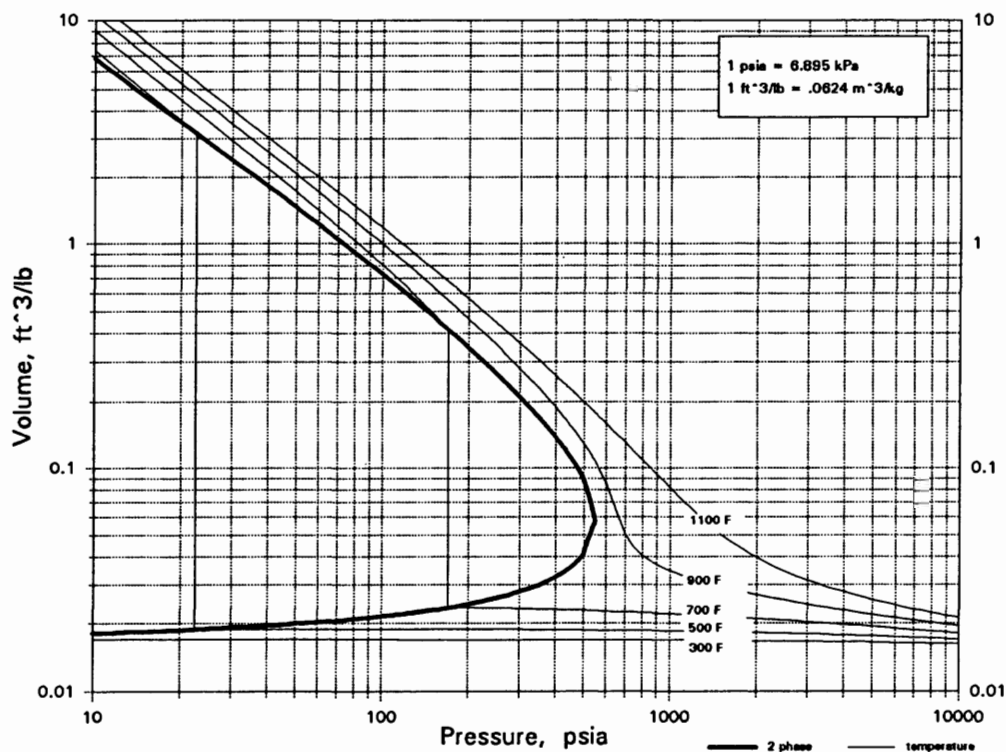


C7H7NO2 o-NITROTOLUENE



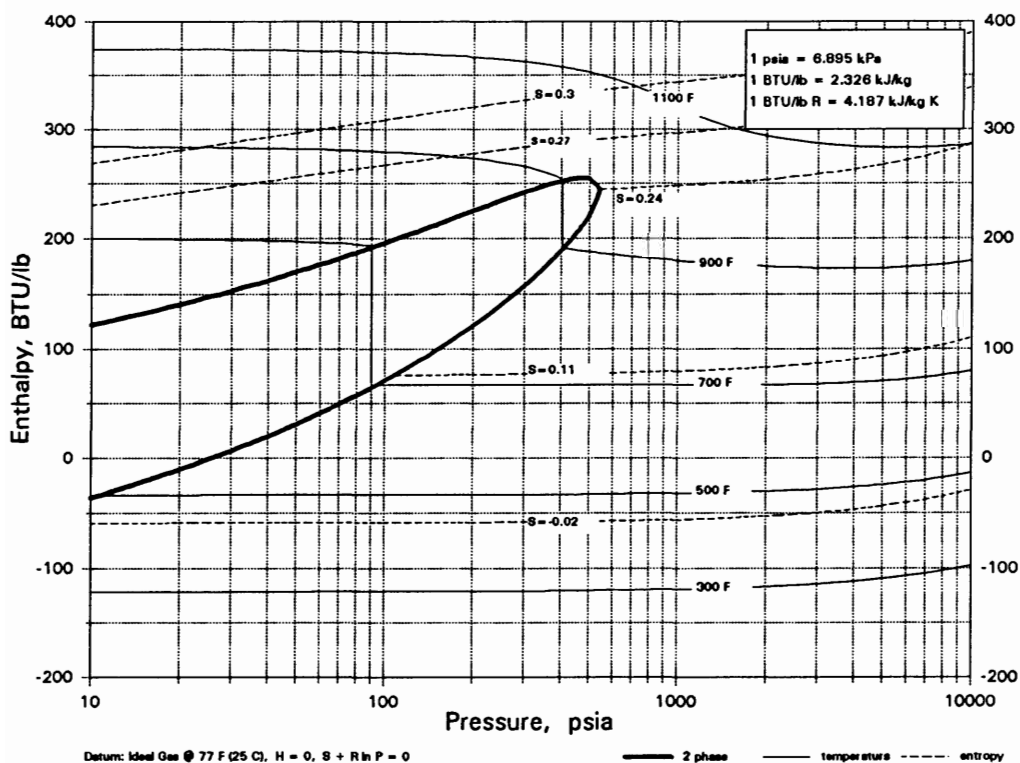
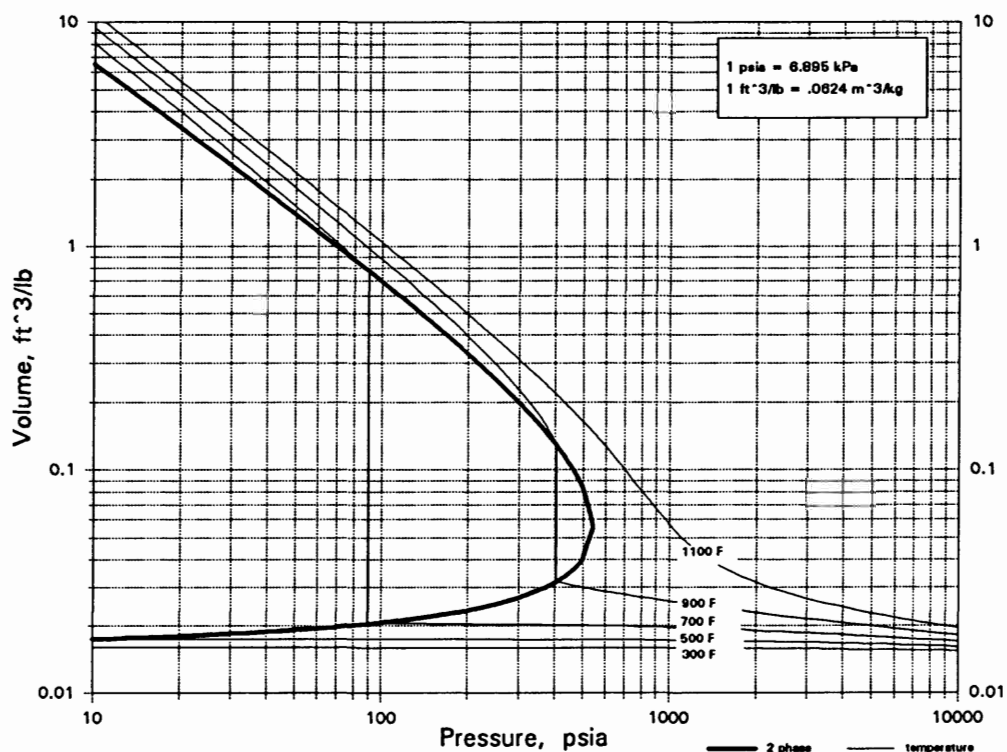
C7H7NO2

p-NITROTOLUENE



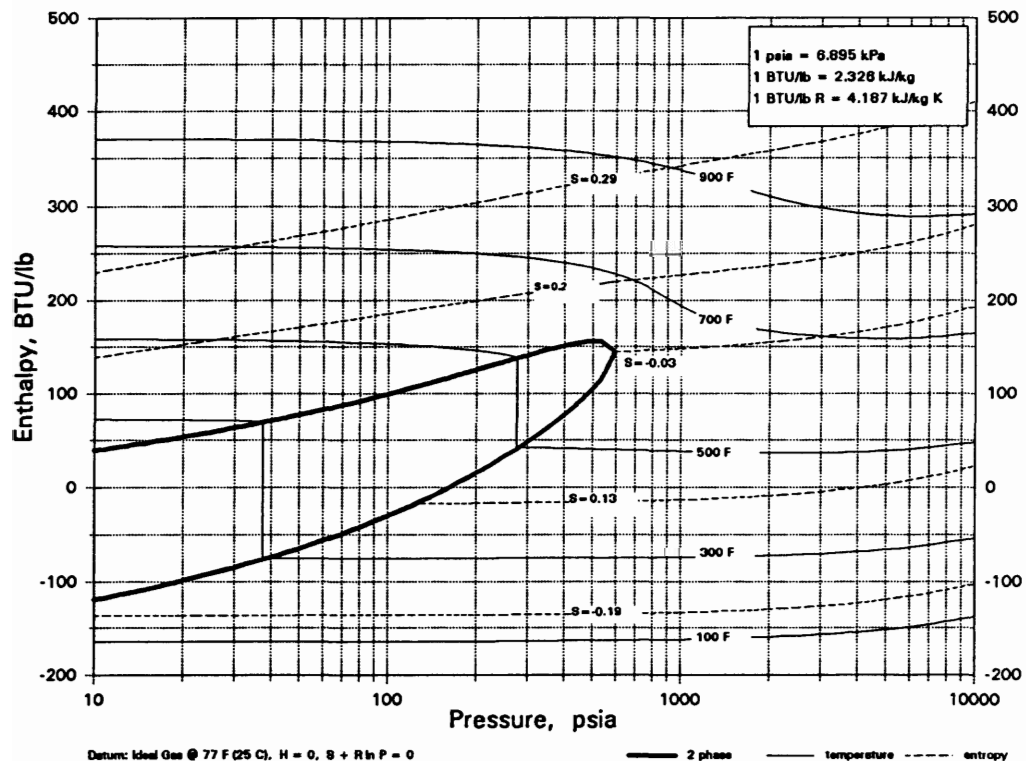
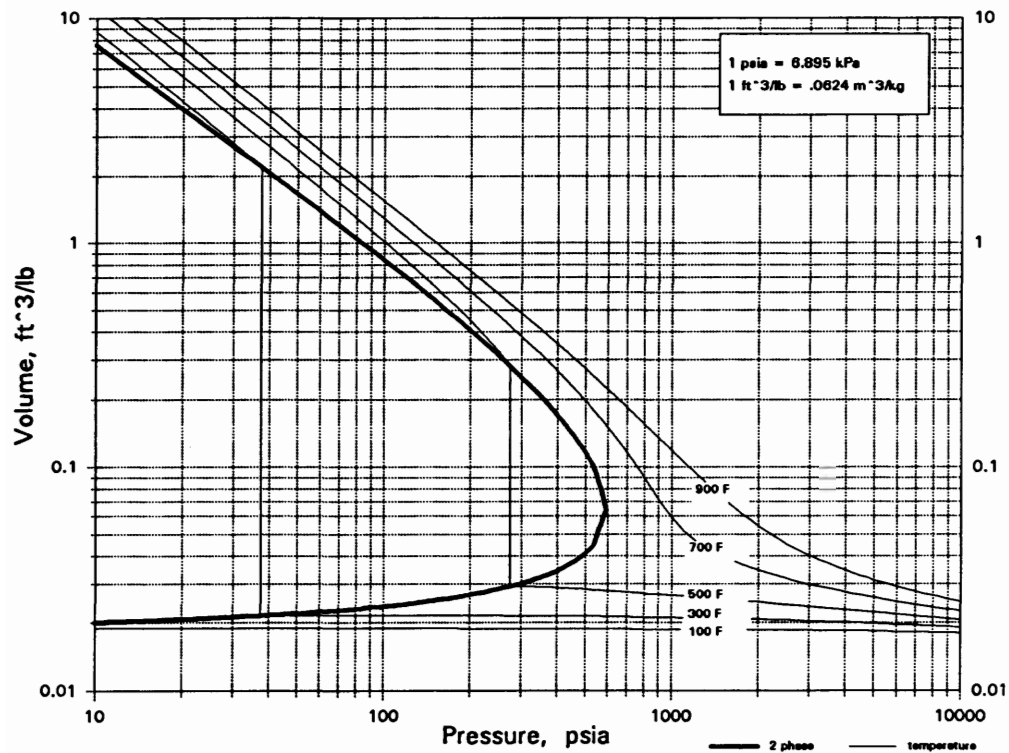
C7H7NO3

o-NITROANISOLE



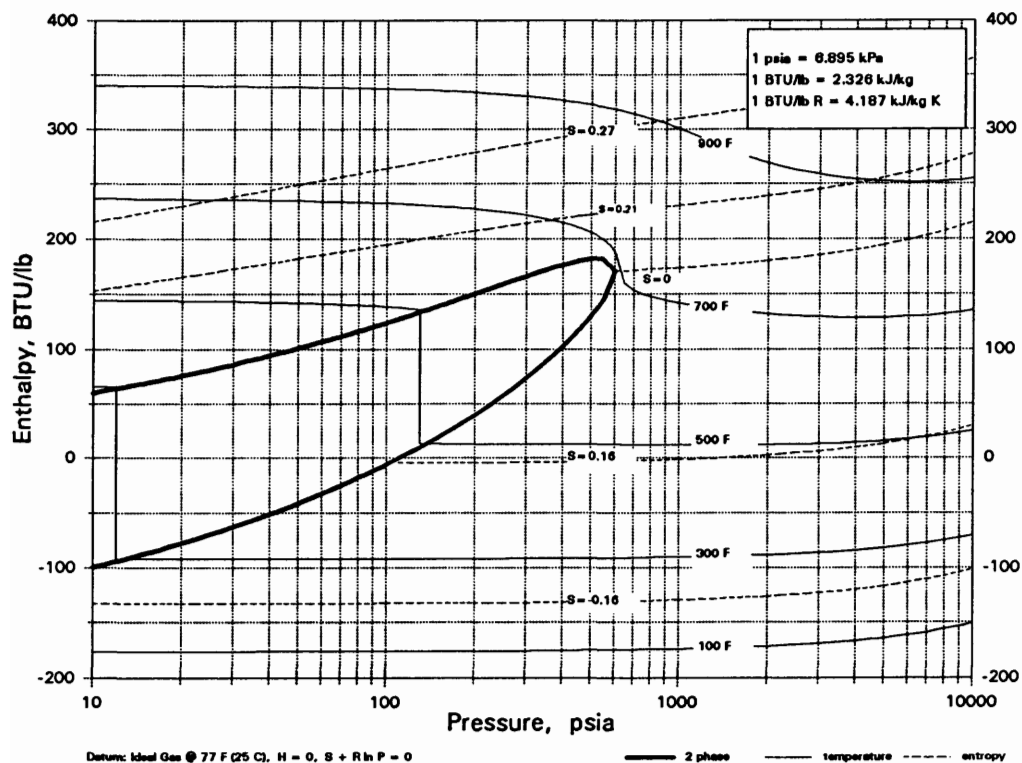
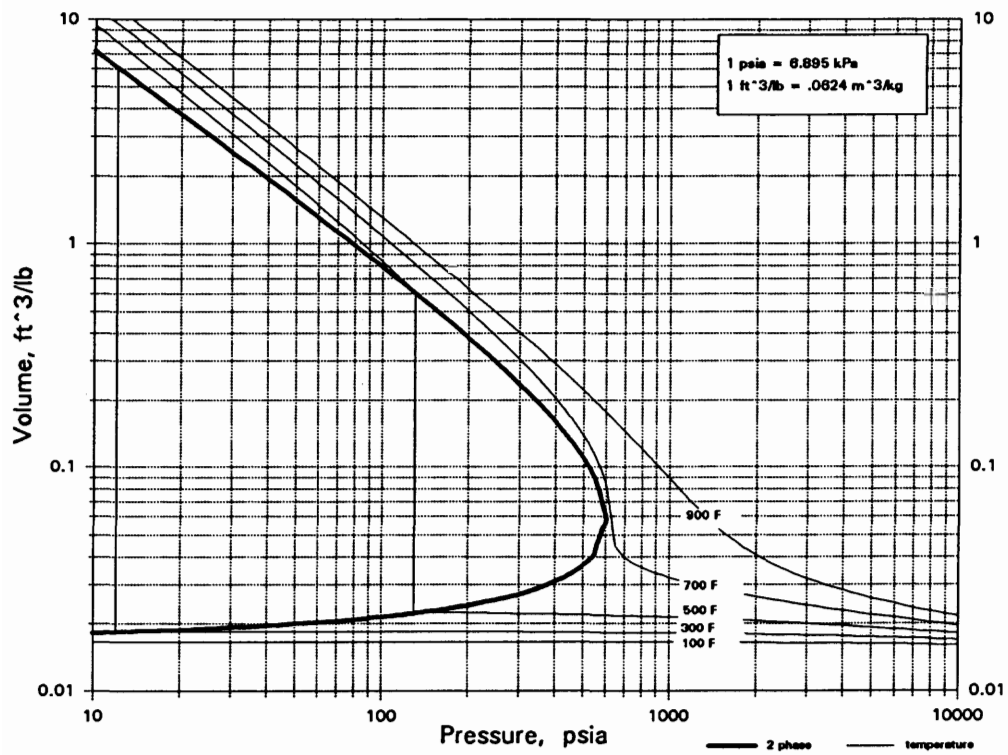
C7H8

TOLUENE



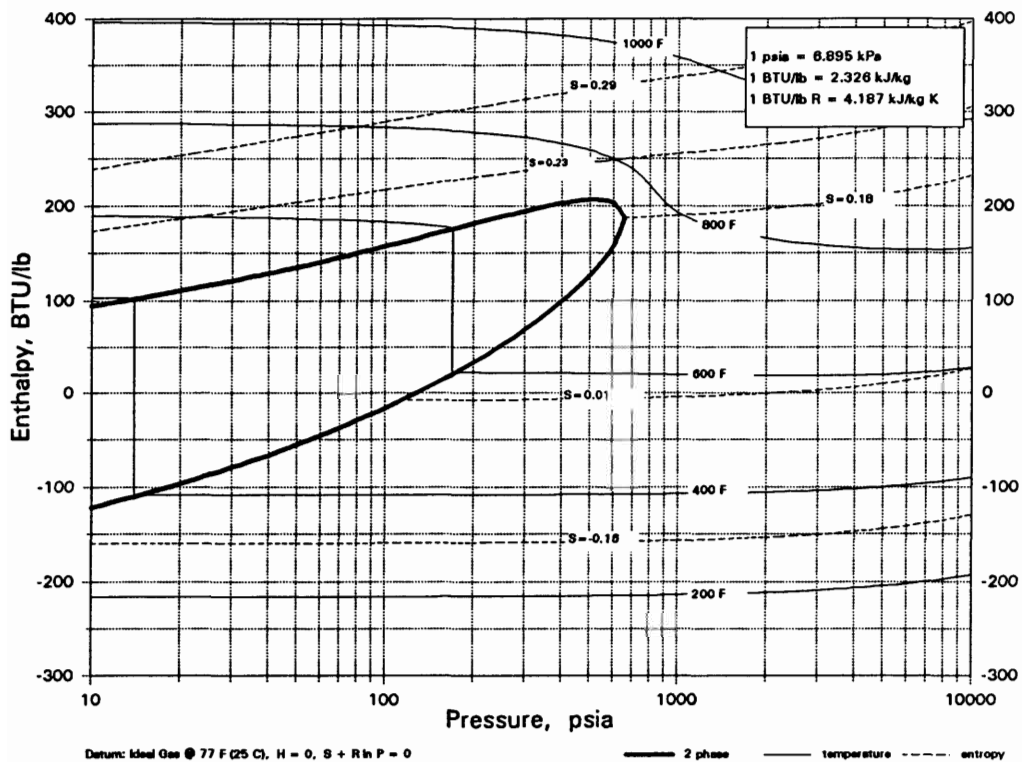
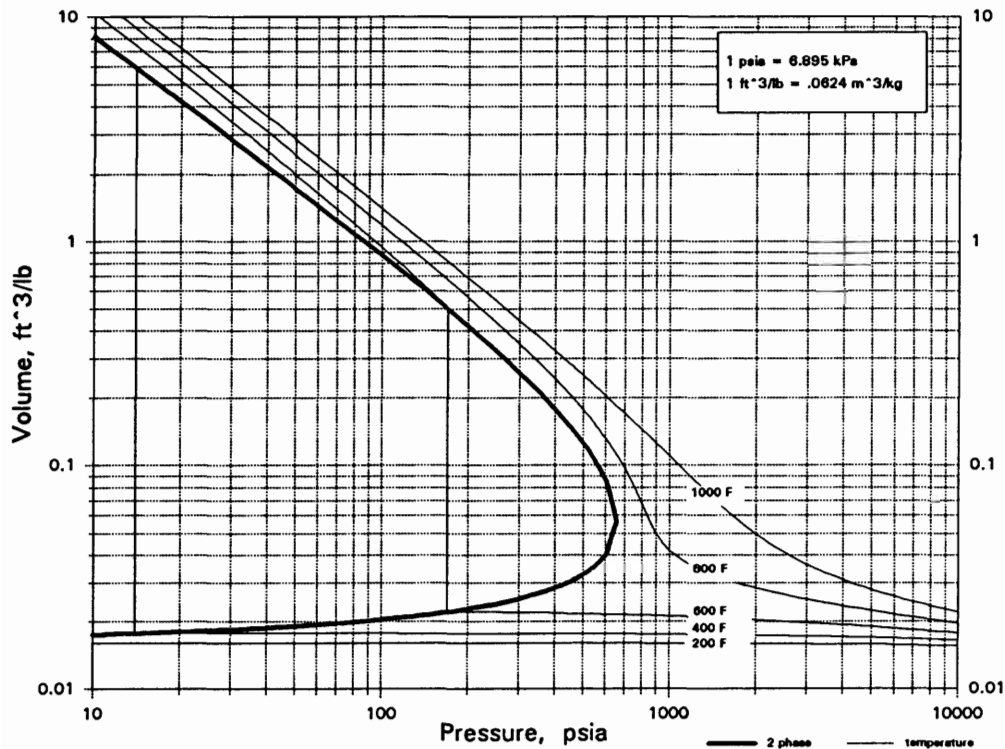
C7H8O

ANISOLE

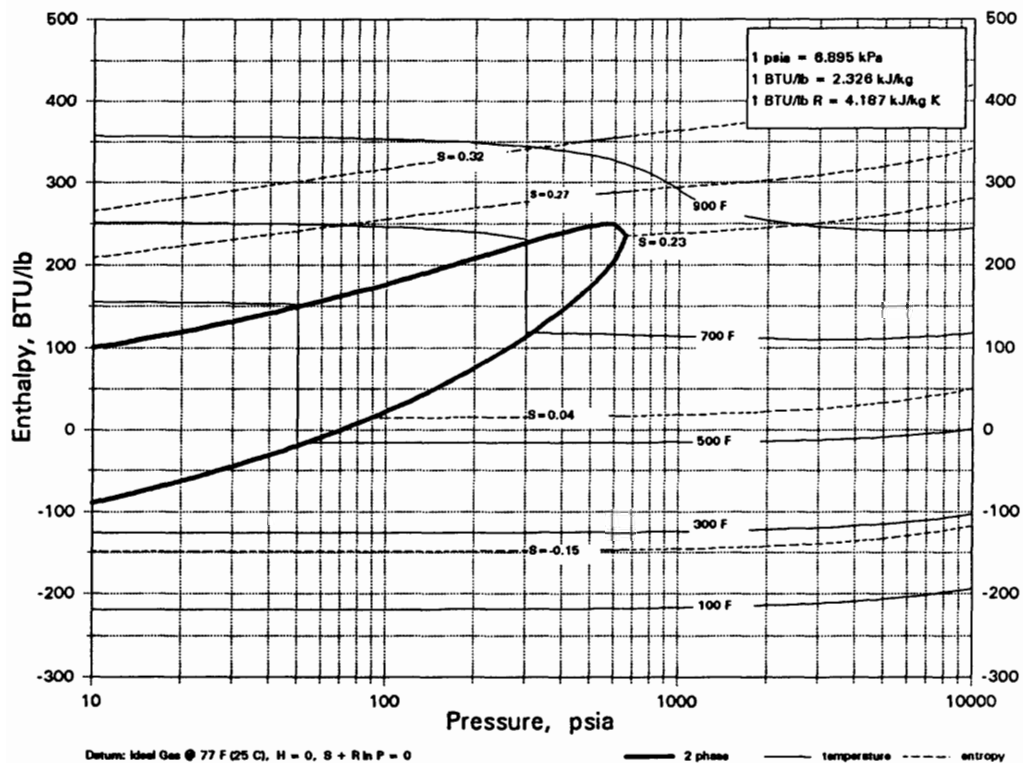
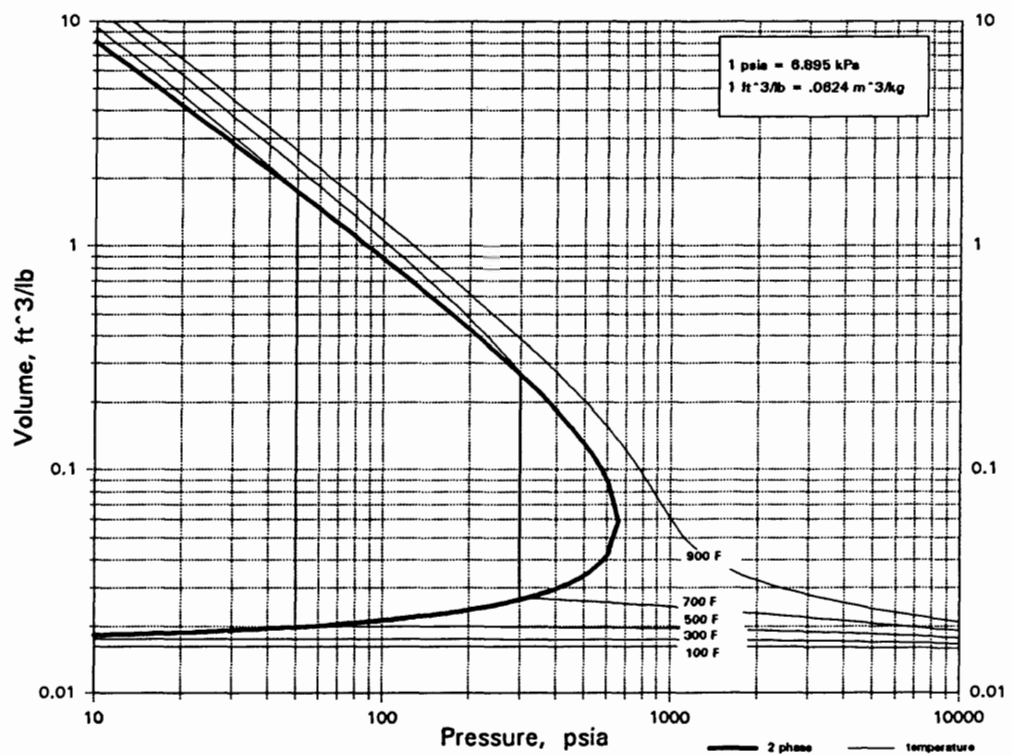


C7H8O

BENZYL ALCOHOL

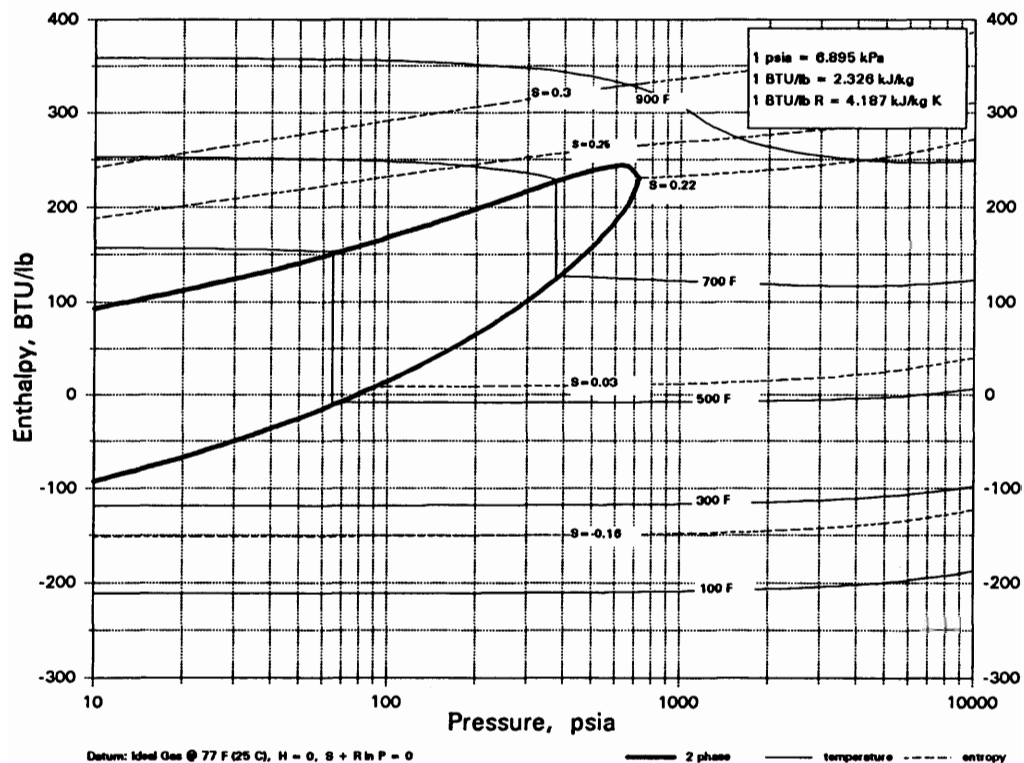
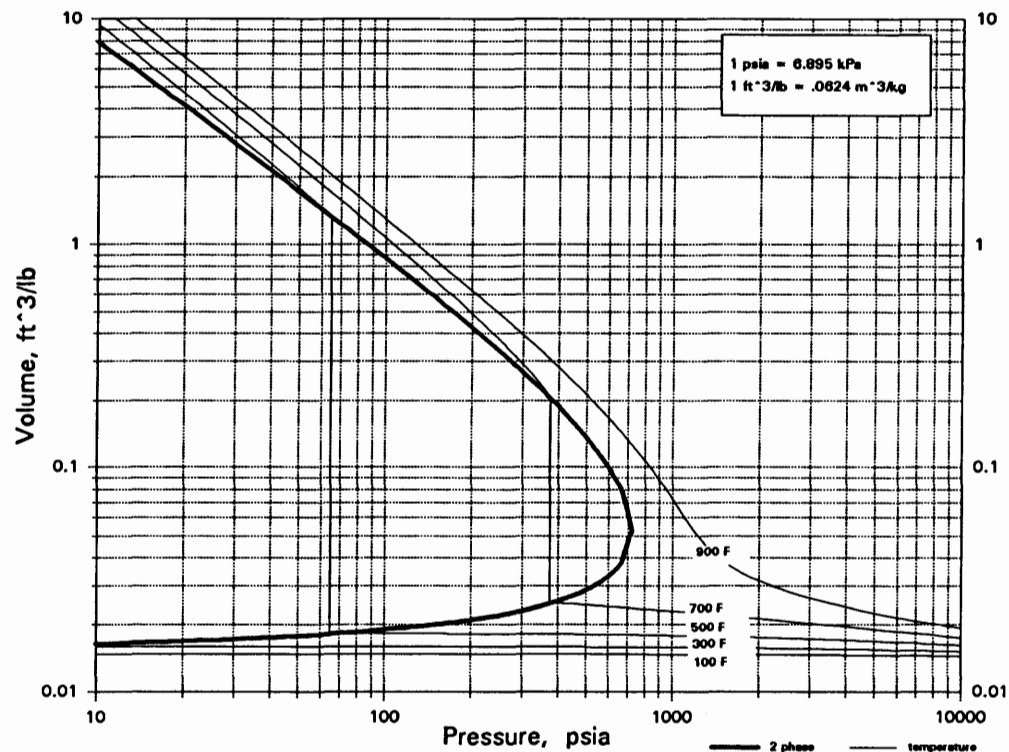


C7H8O
m-CRESOL



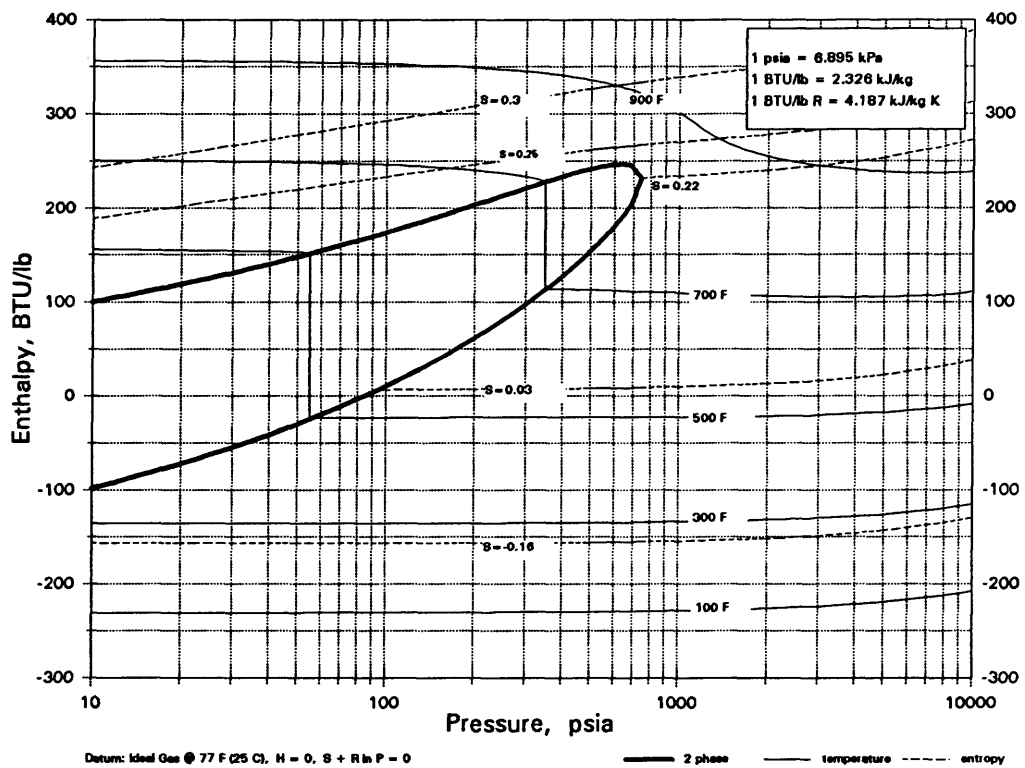
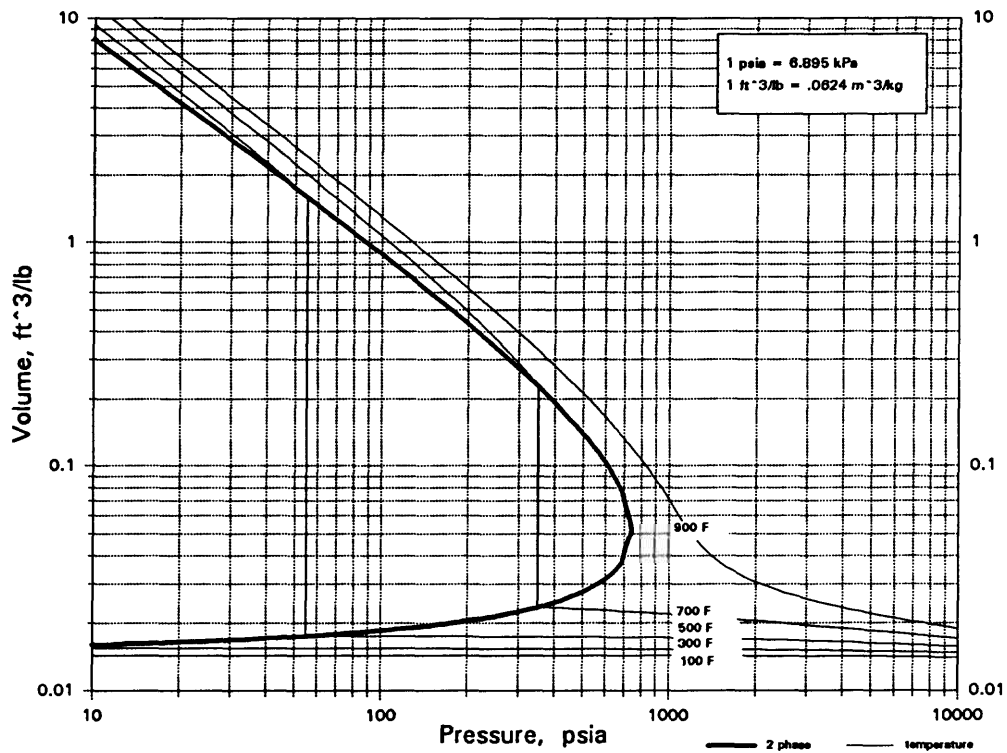
C7H8O

o-CRESOL



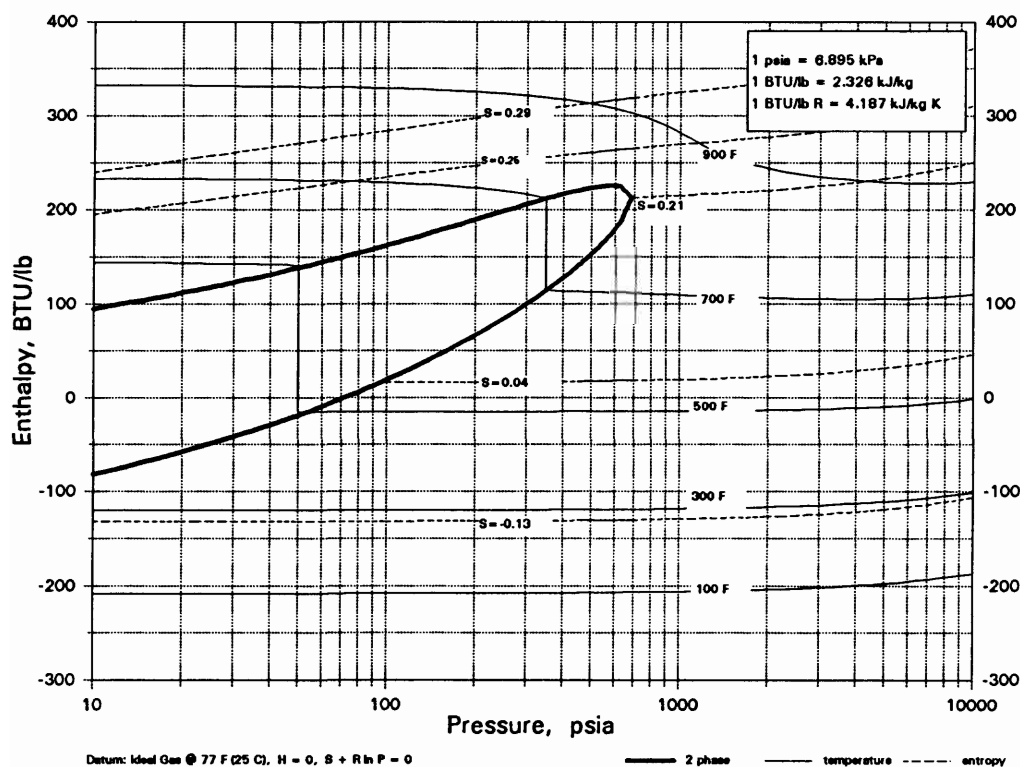
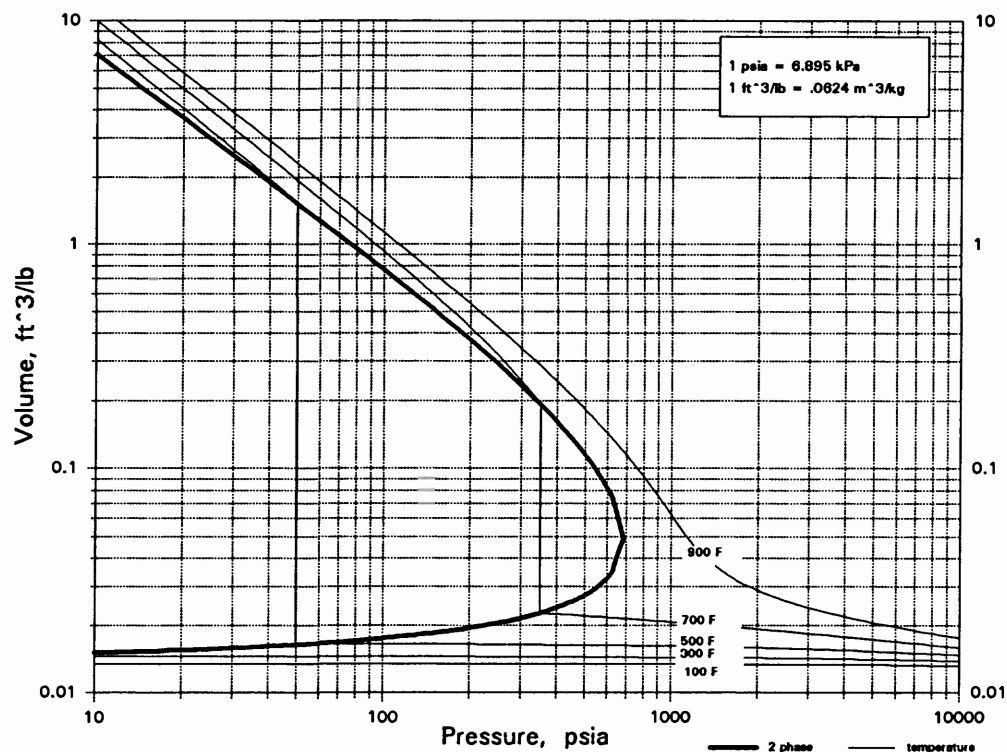
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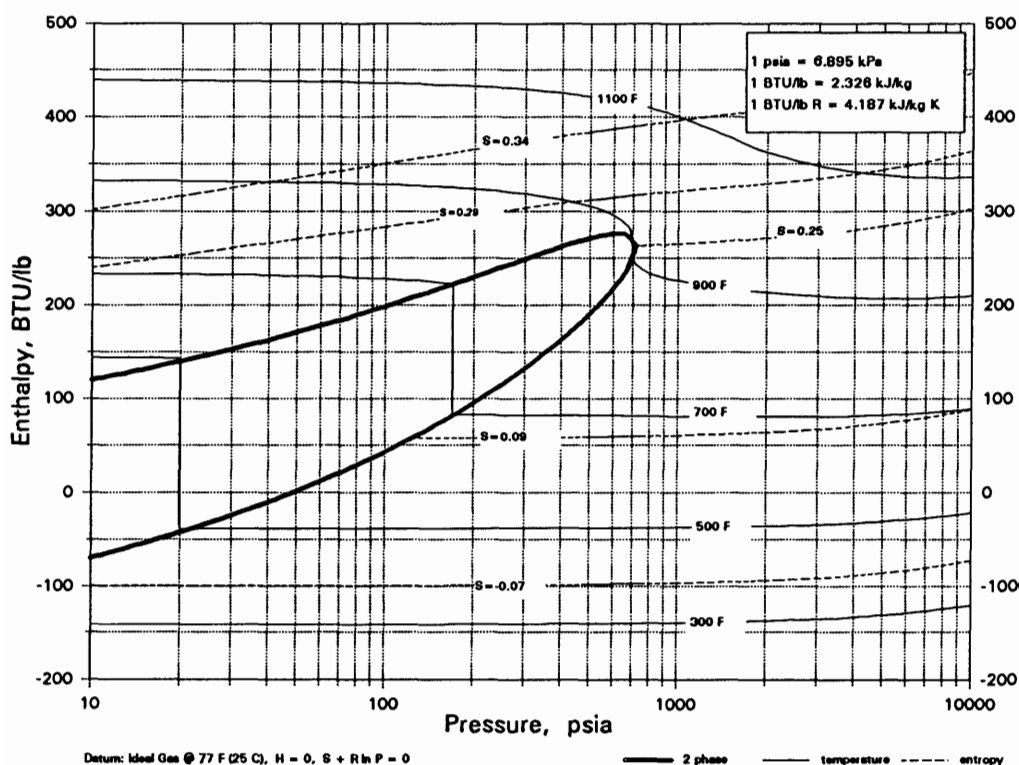
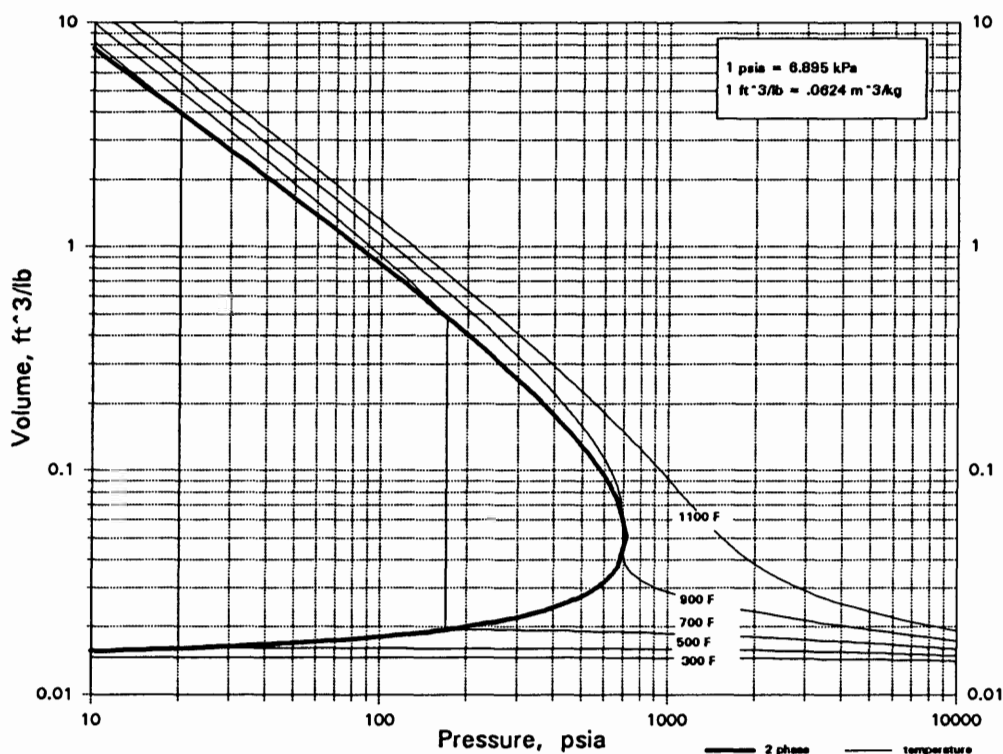
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GUAIACOL



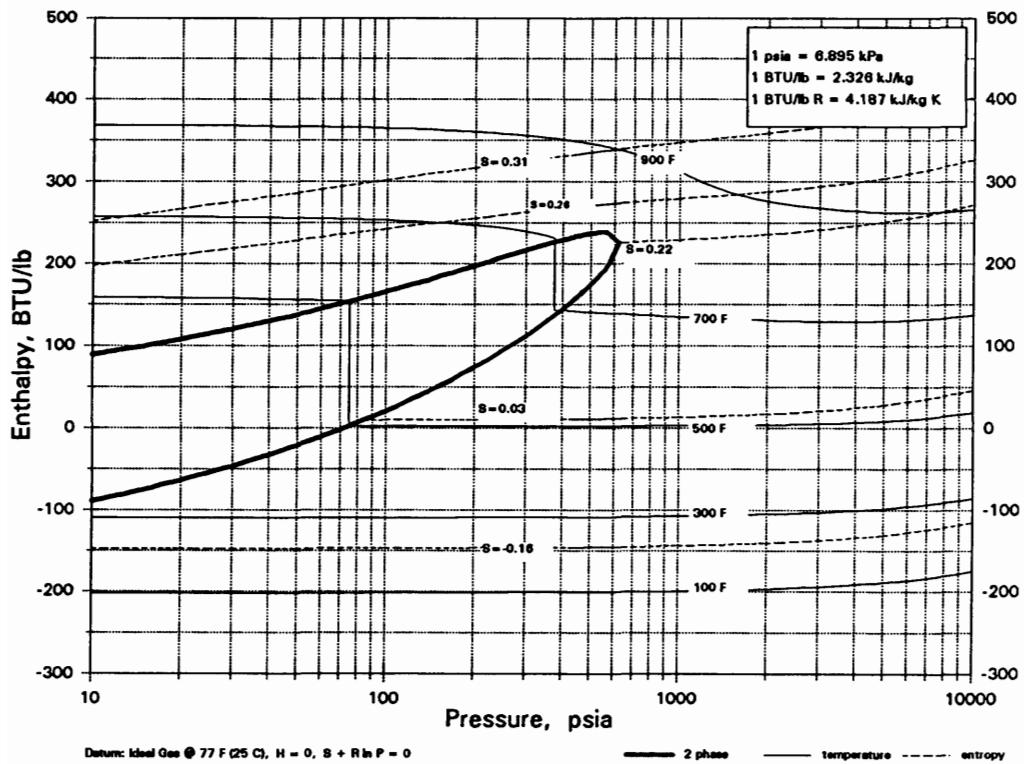
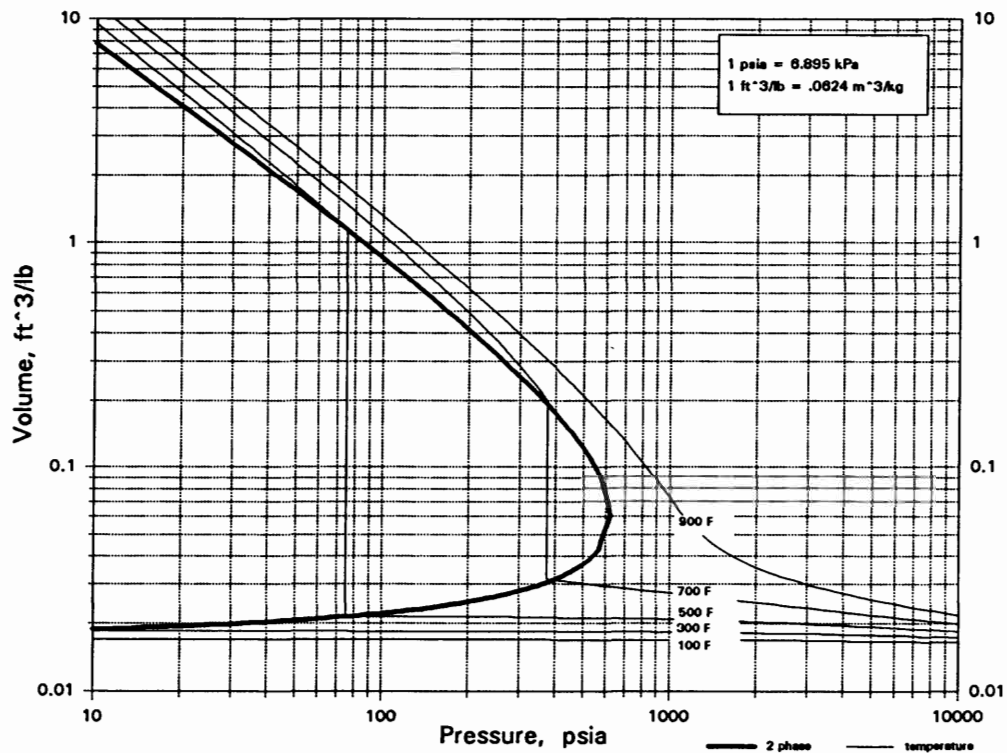
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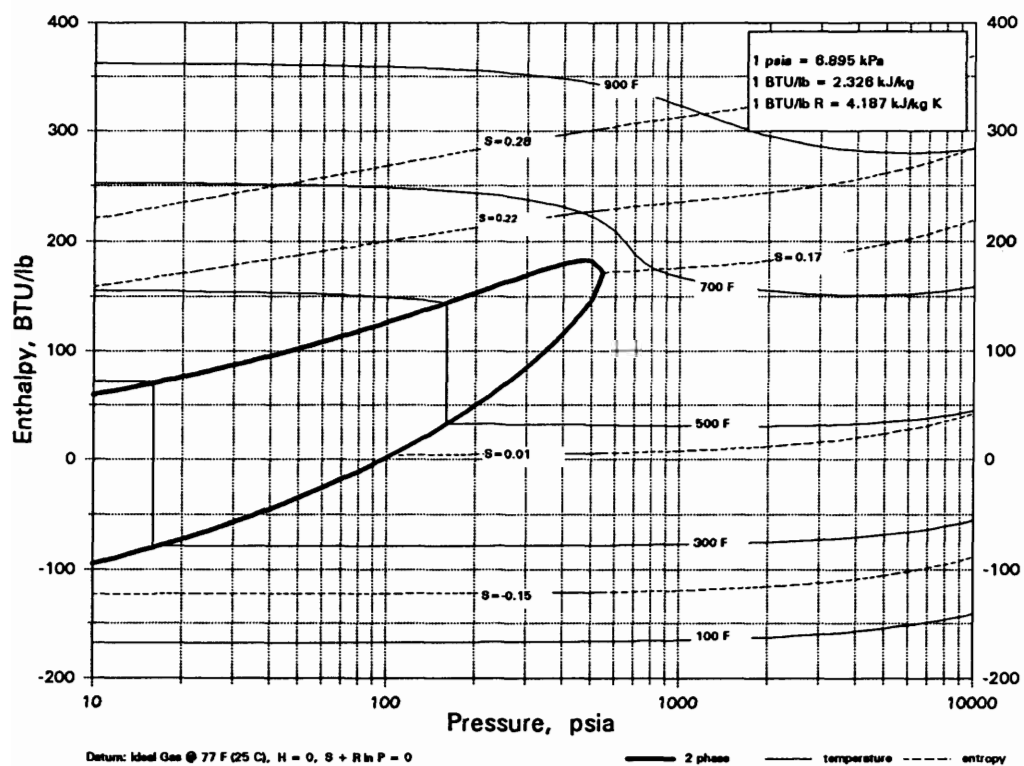
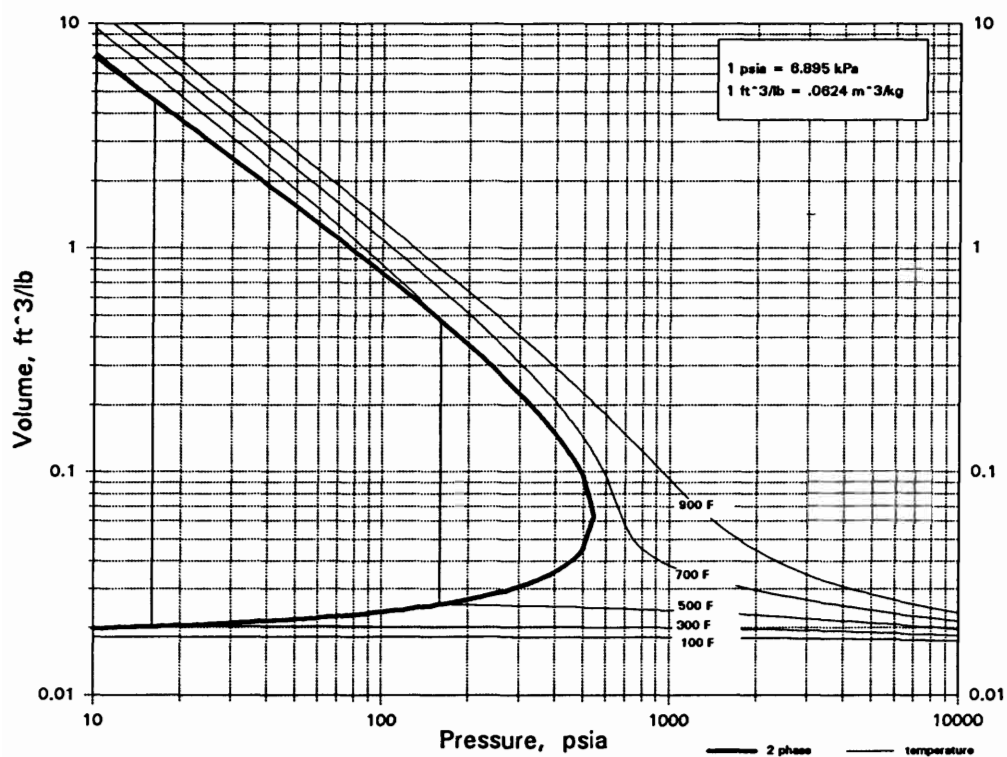
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BENZYLAMINE



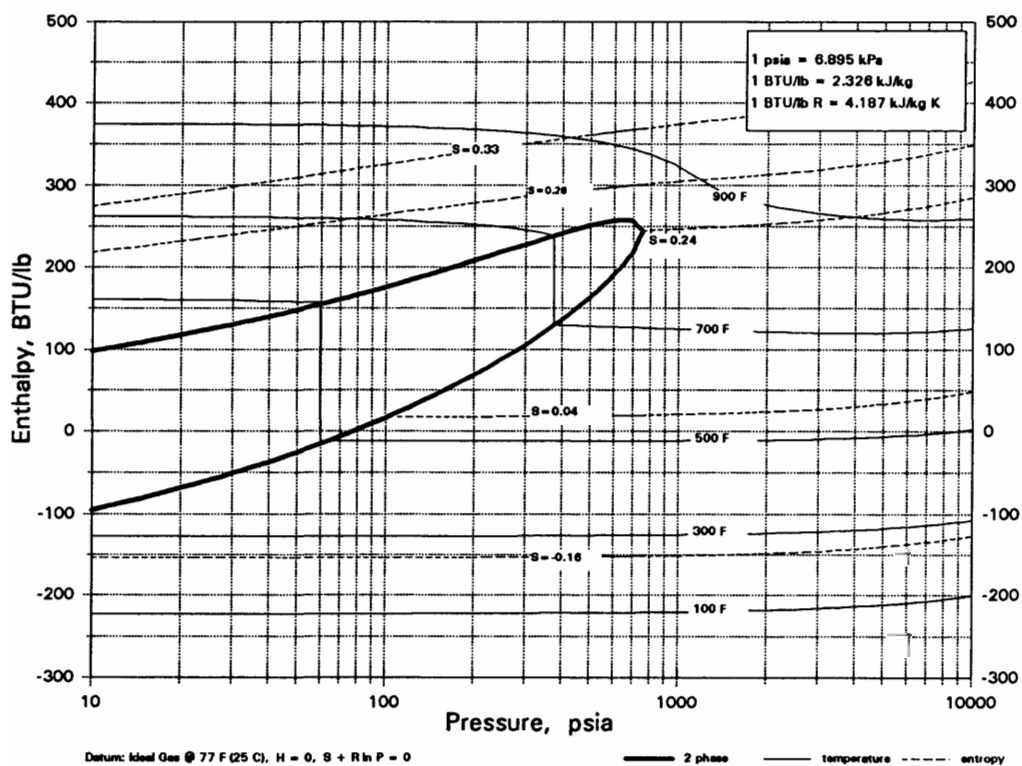
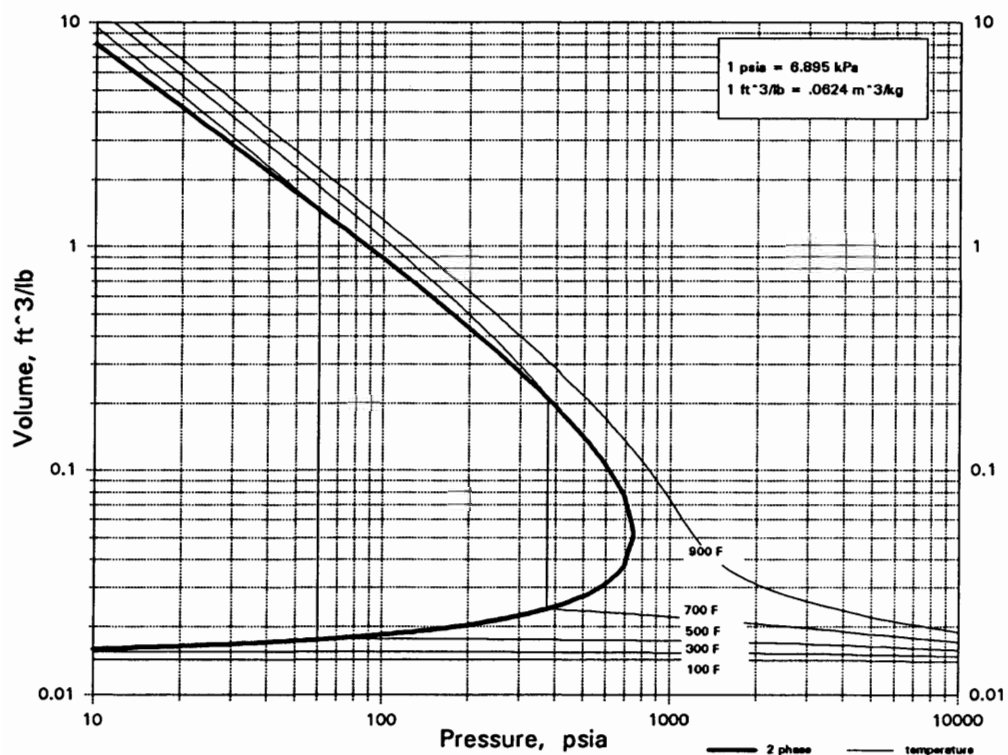
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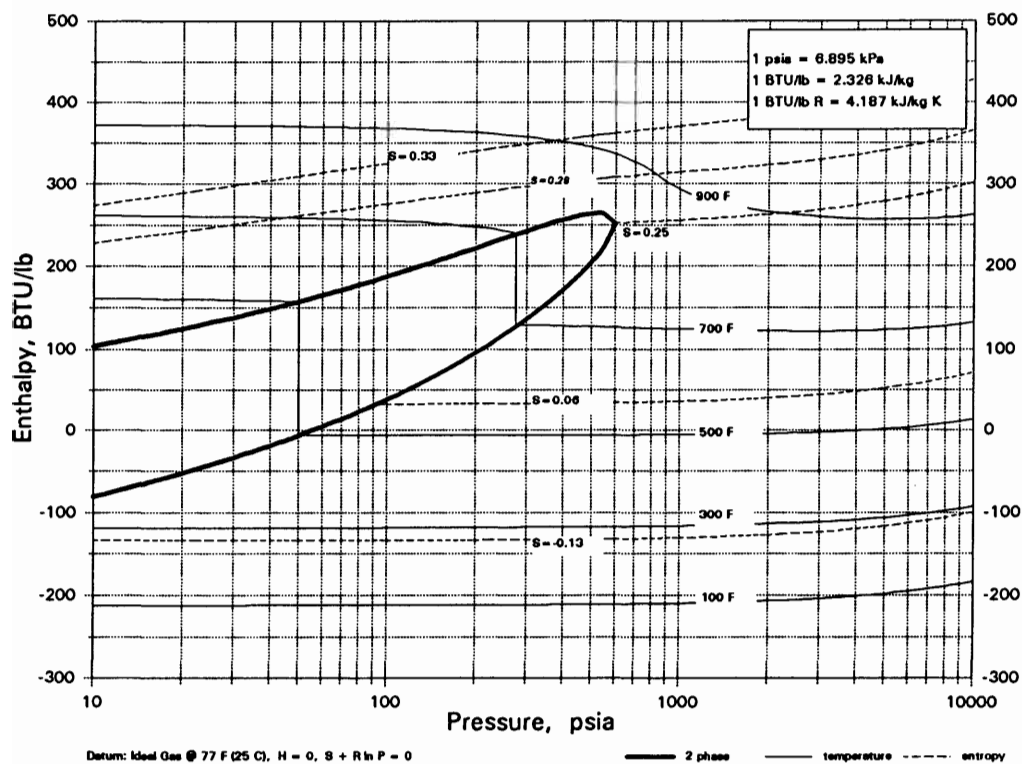
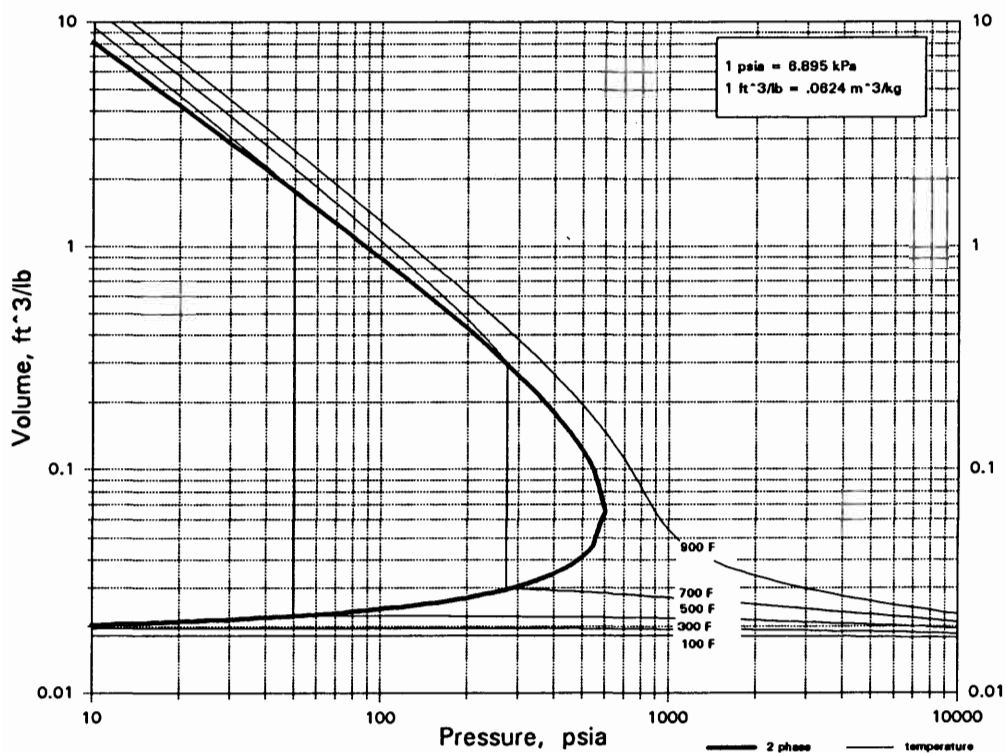
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N-METHYLANILINE



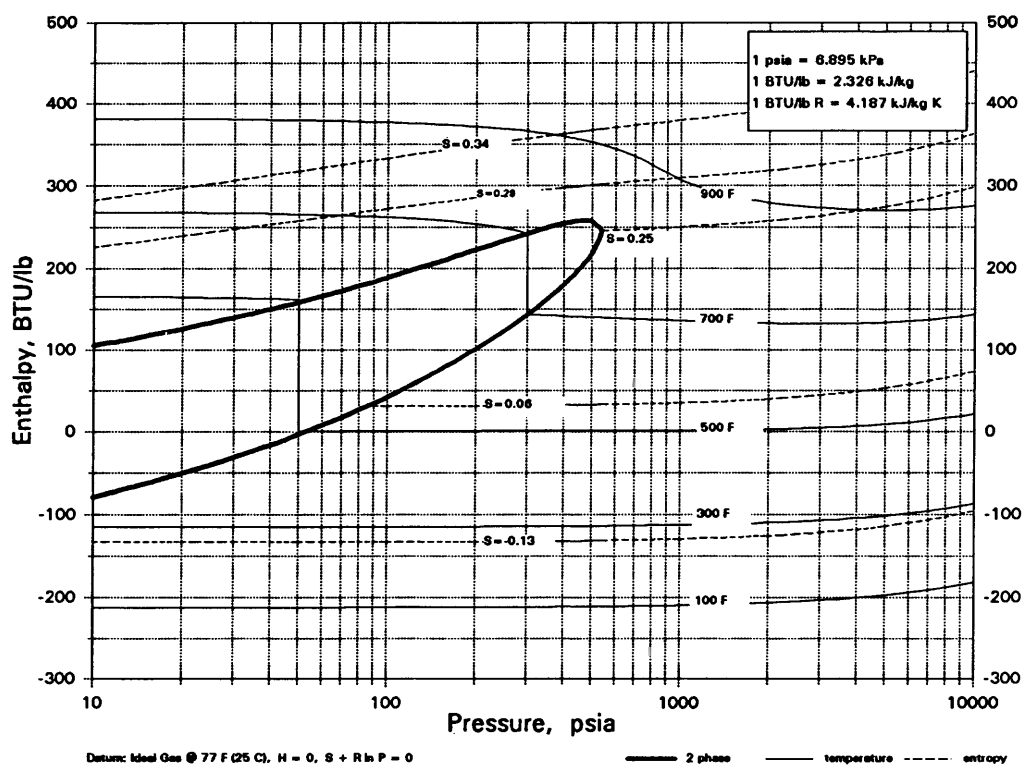
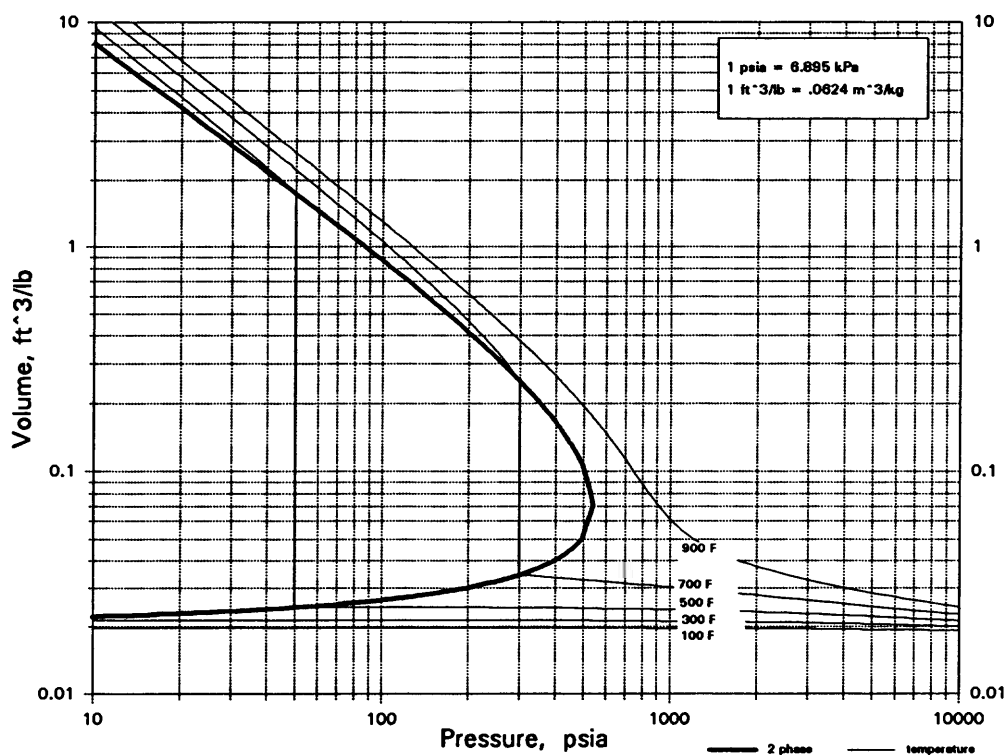
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m-TOLUIDINE



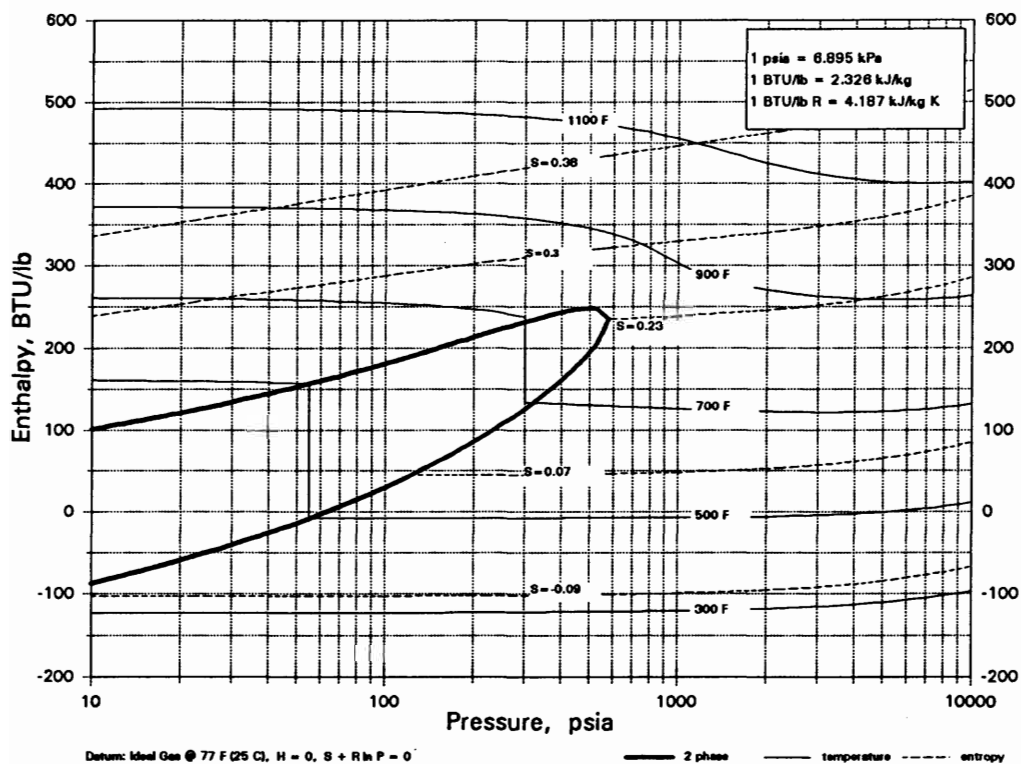
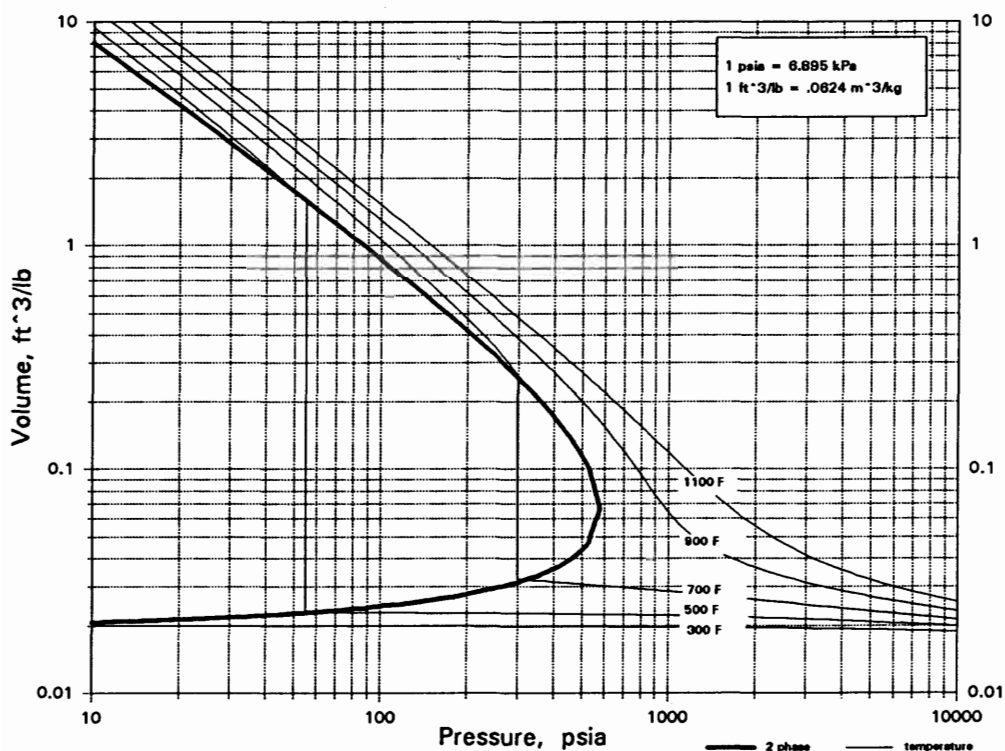
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o-TOLUIDINE



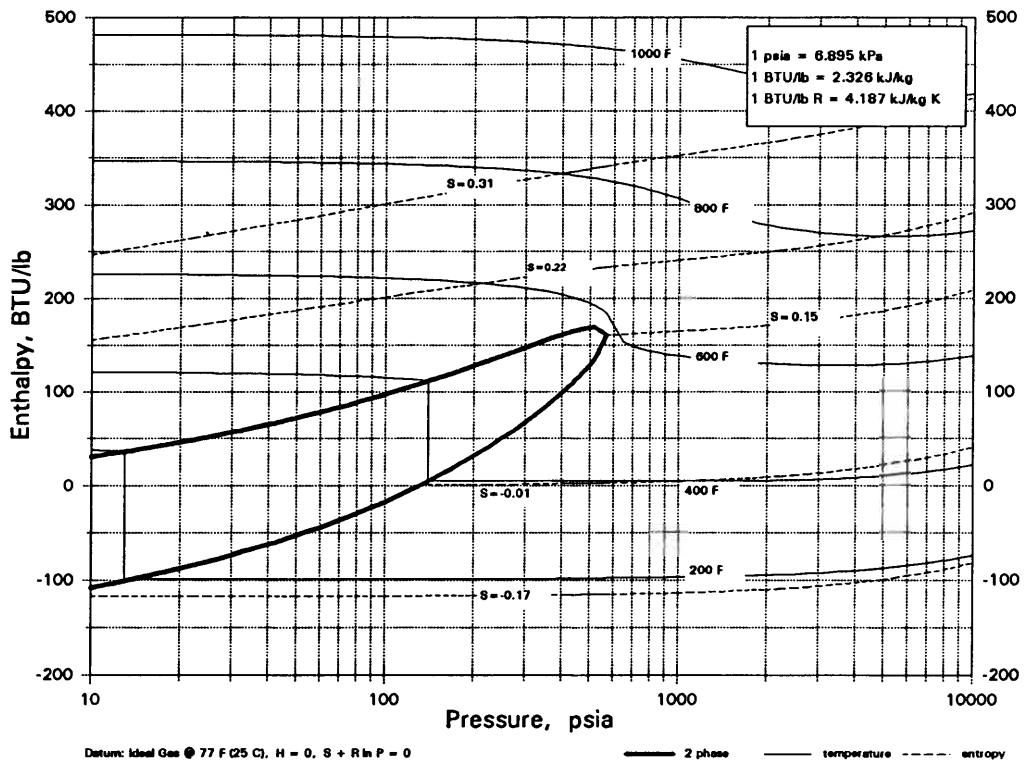
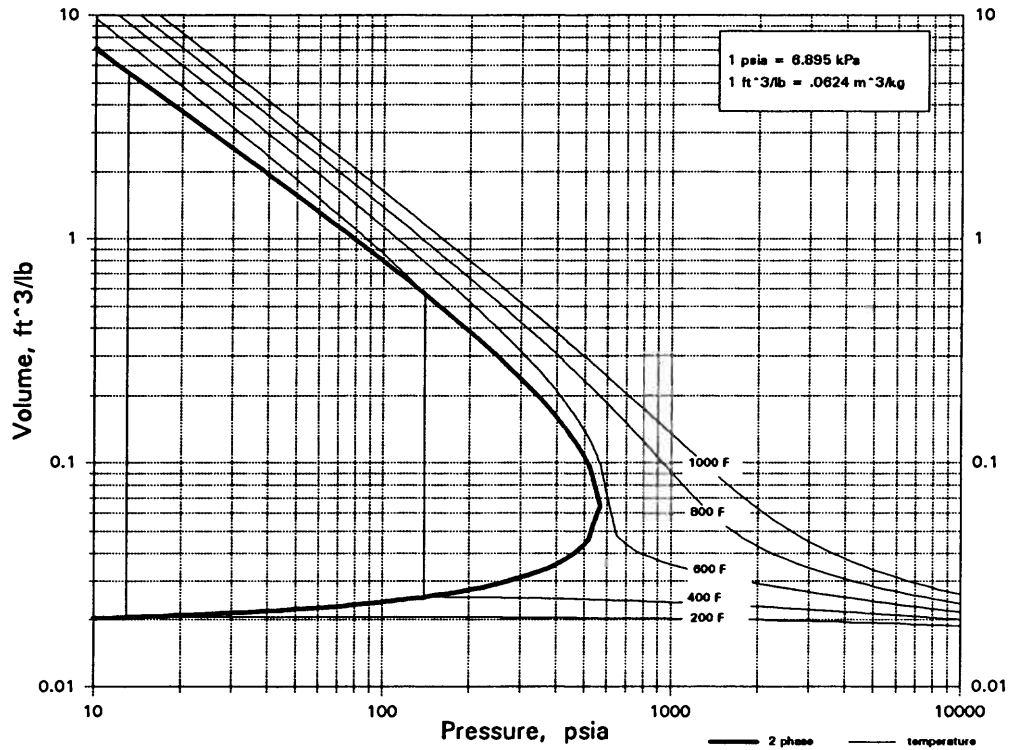
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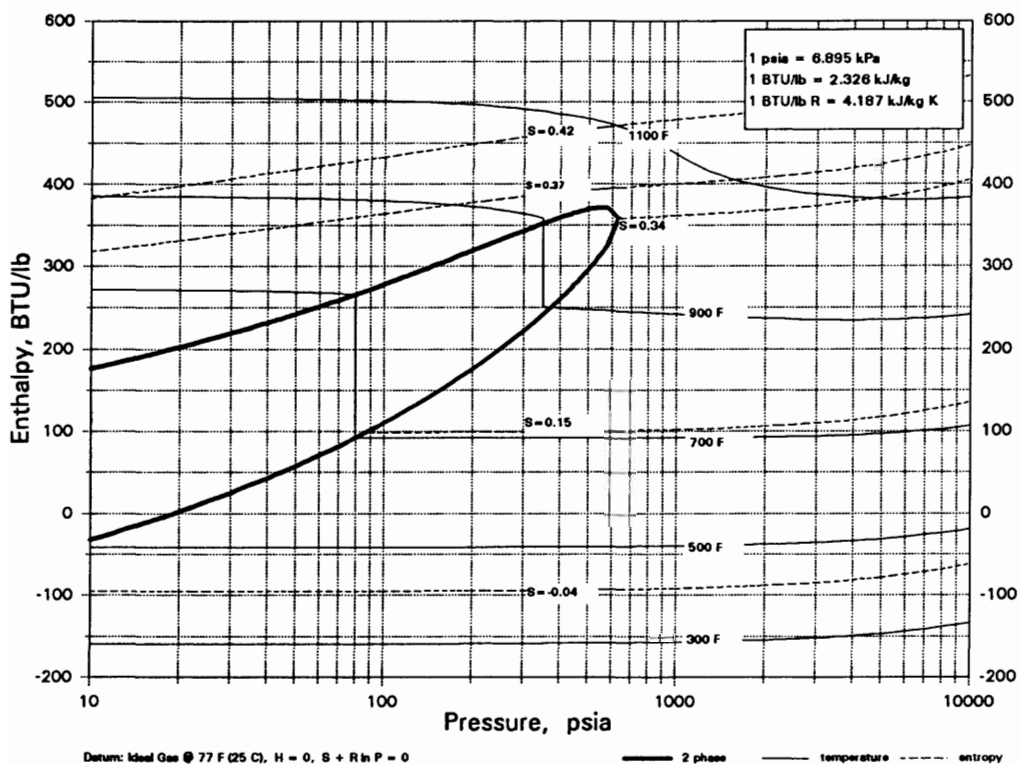
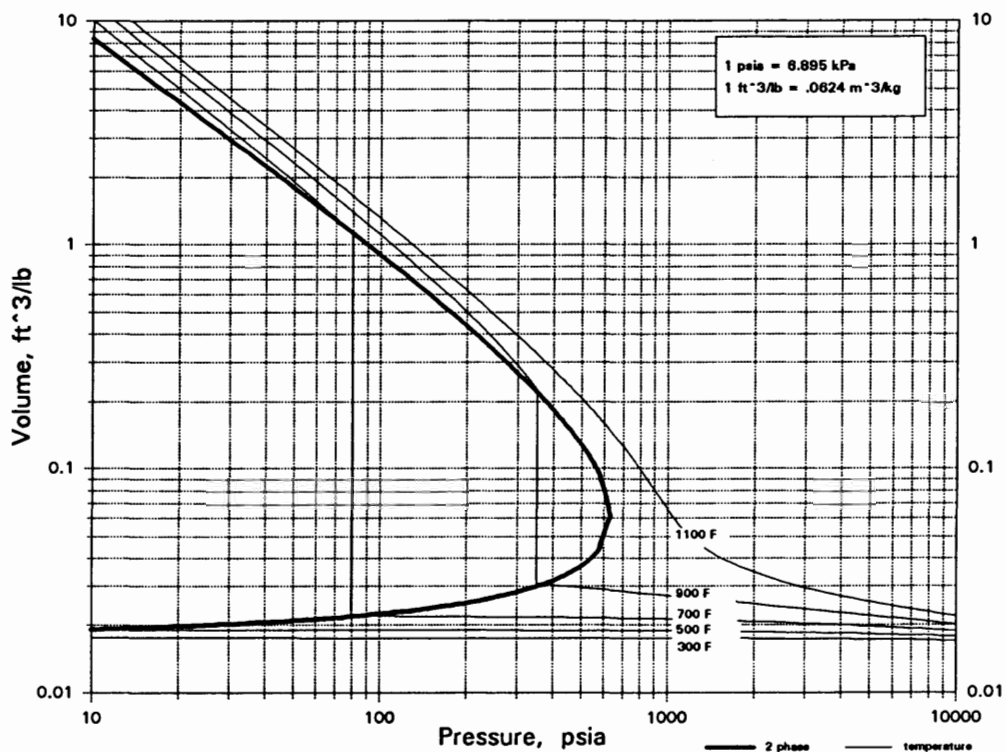
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2-NORBORNENE



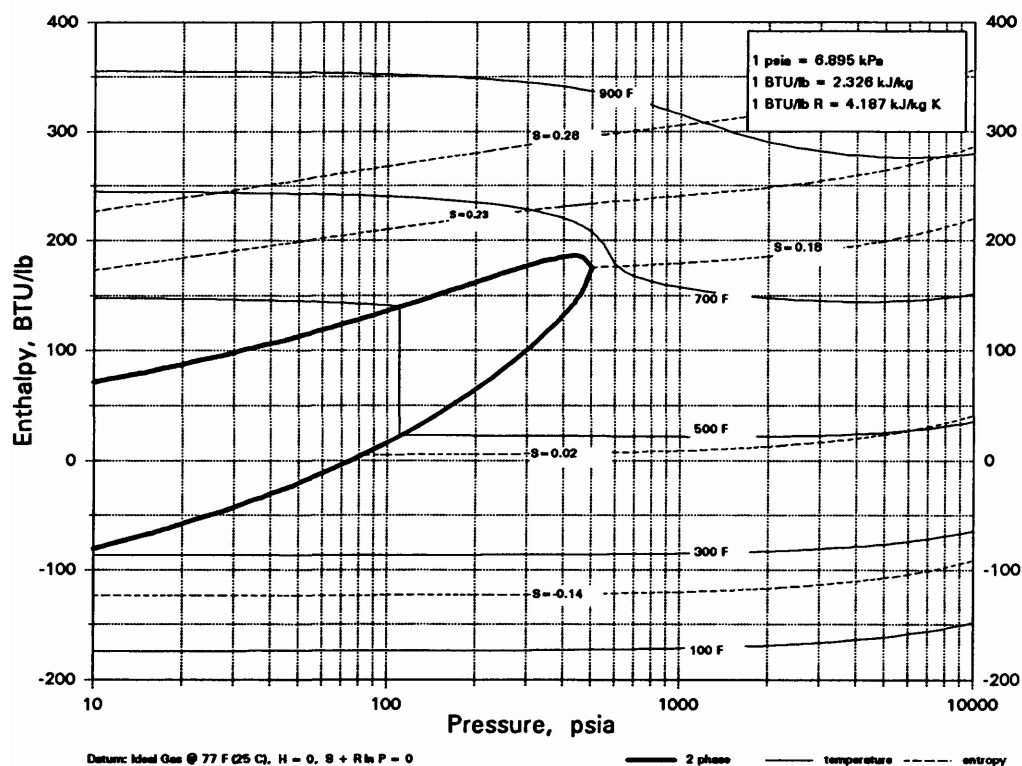
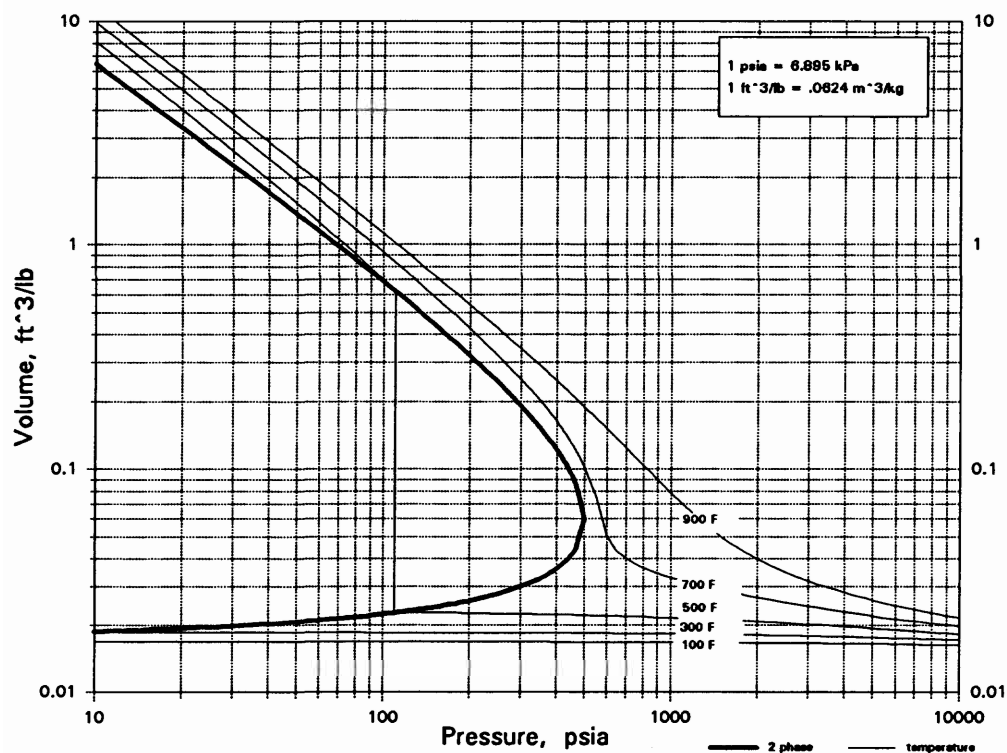
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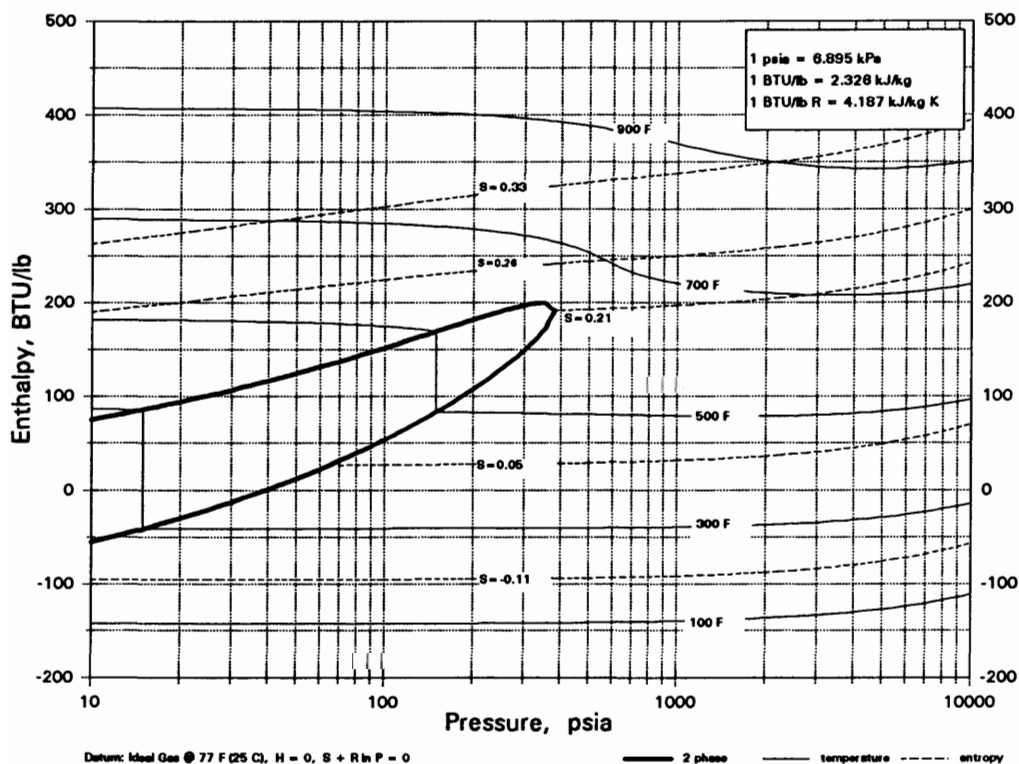
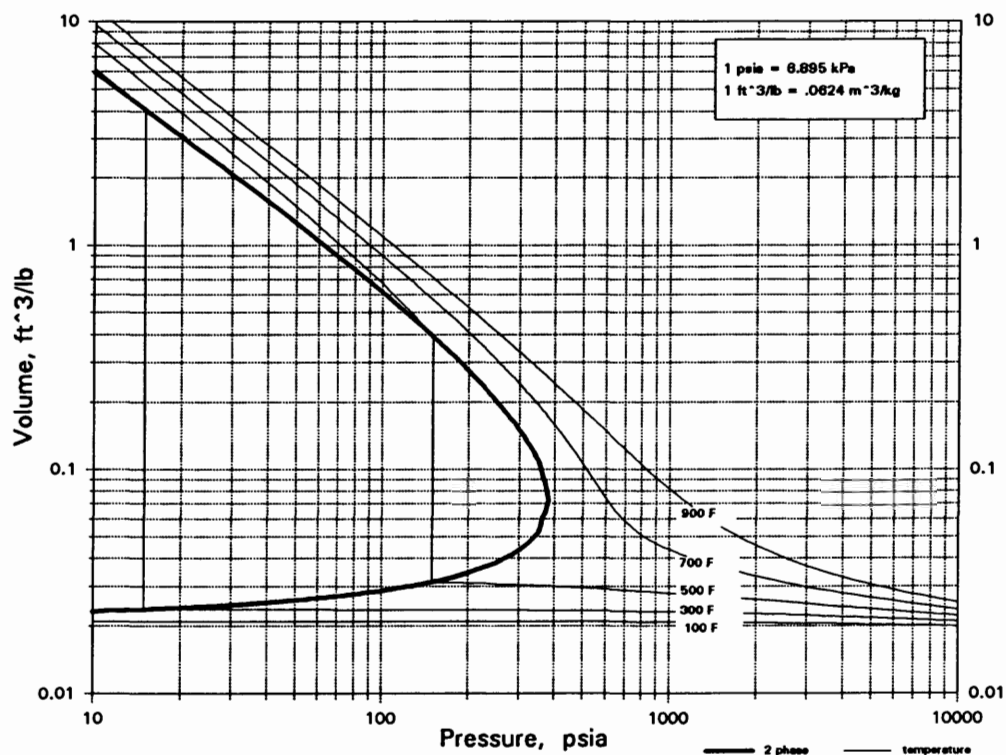
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CYCLOHEXYL ISOCYANATE



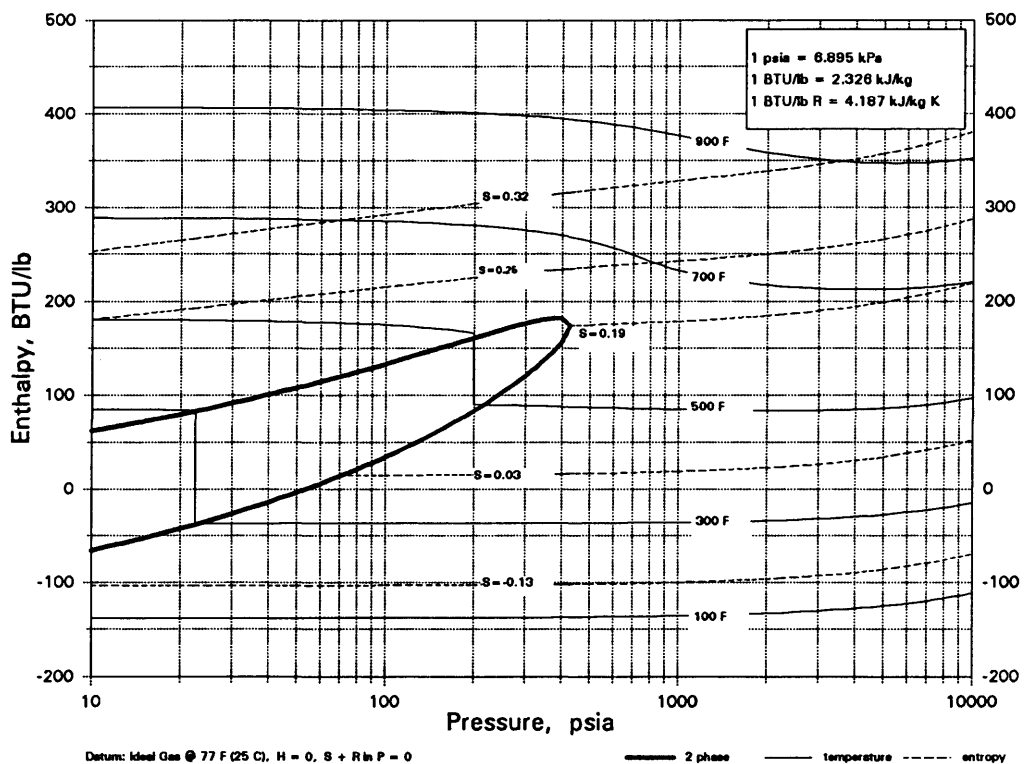
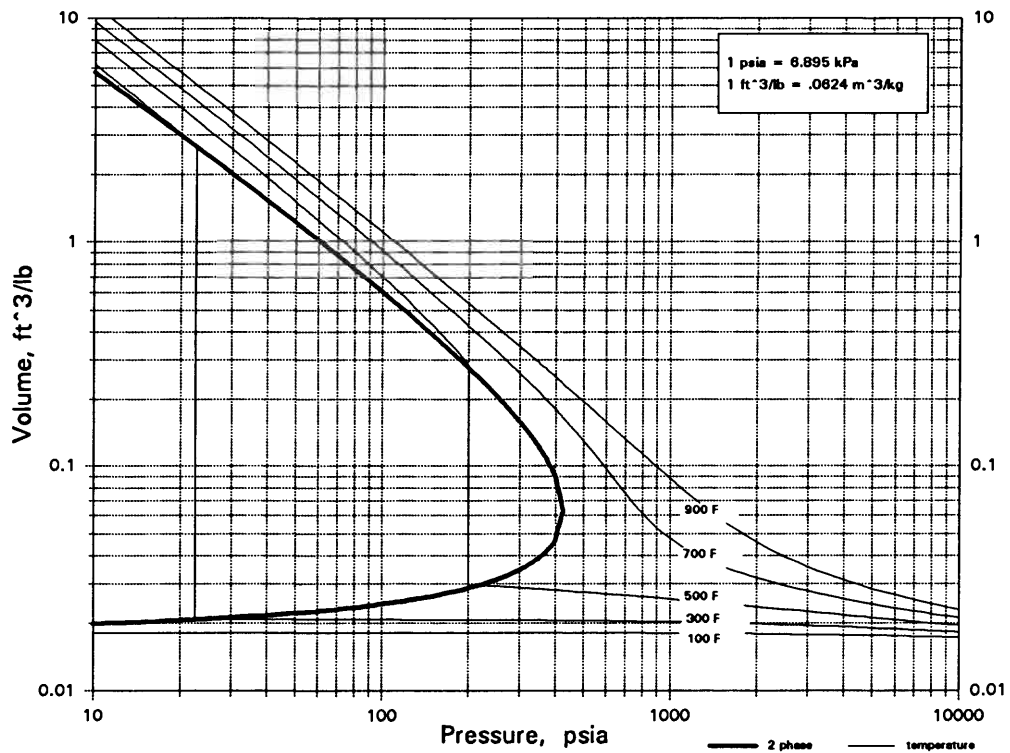
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n-BUTYL ACRYLATE



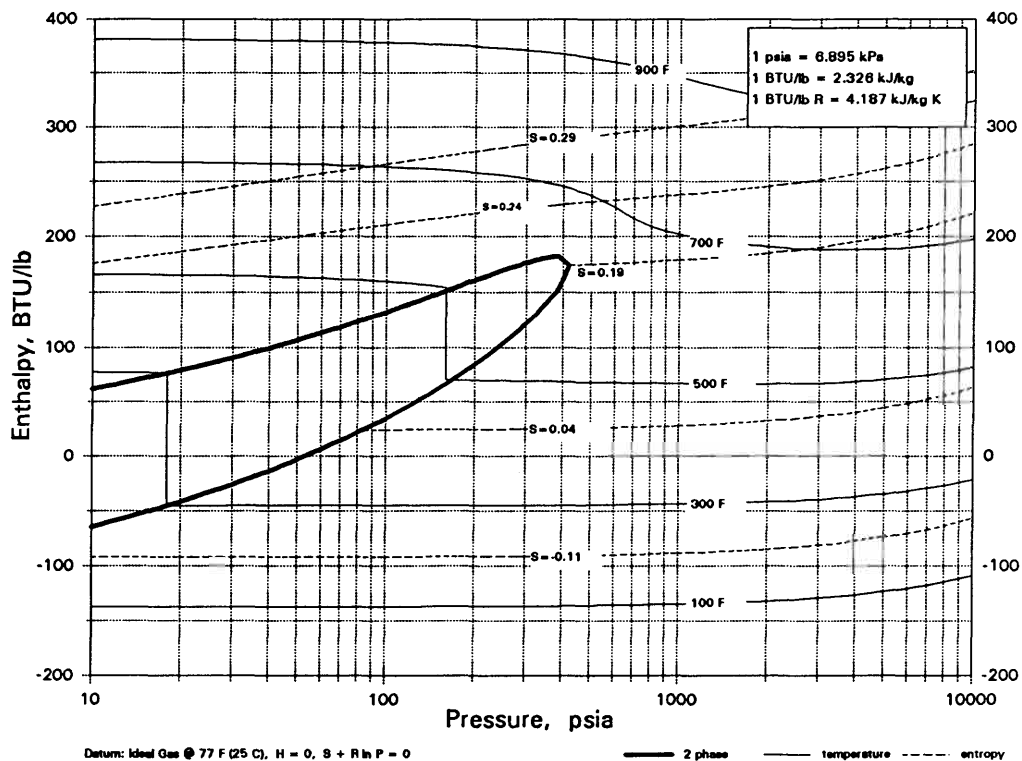
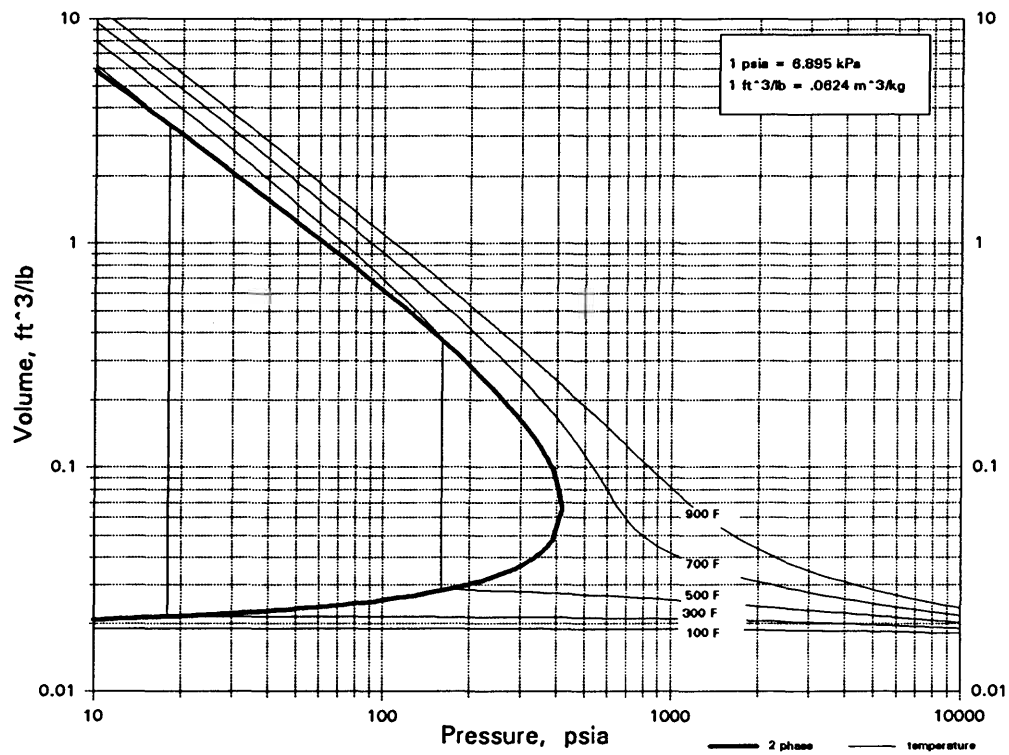
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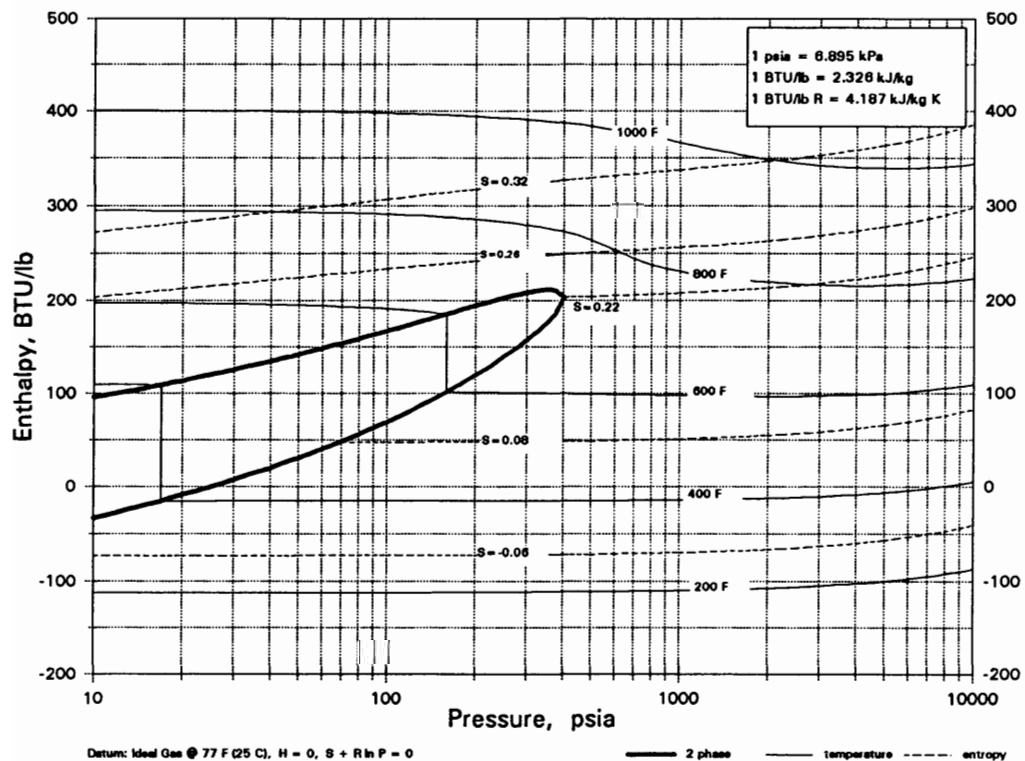
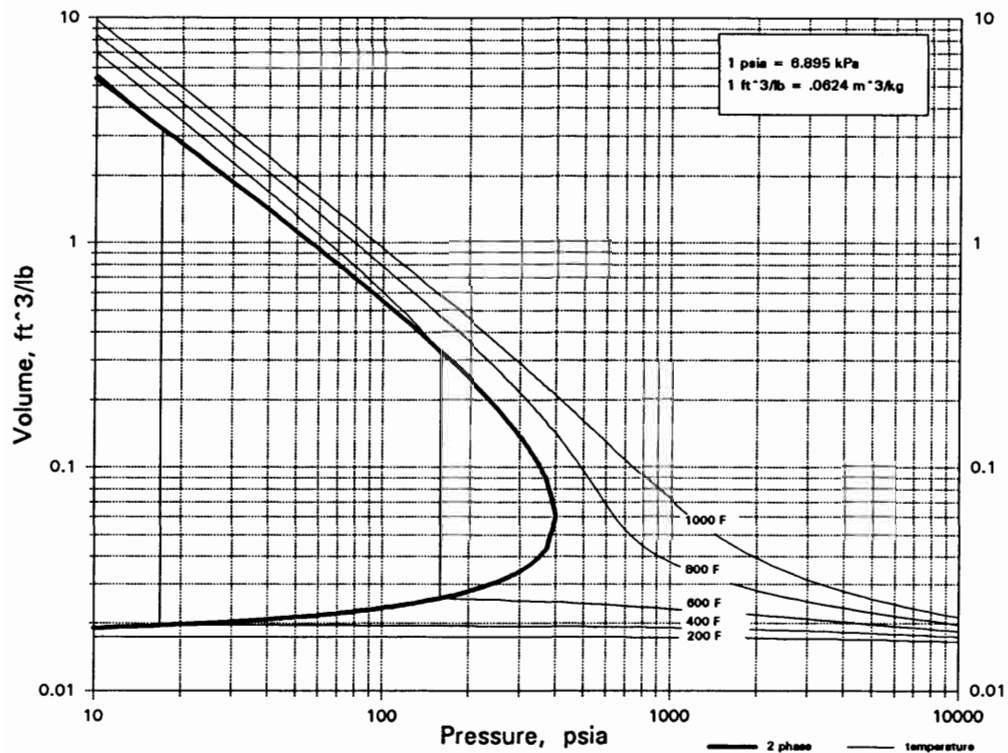
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n-PROPYL METHACRYLATE



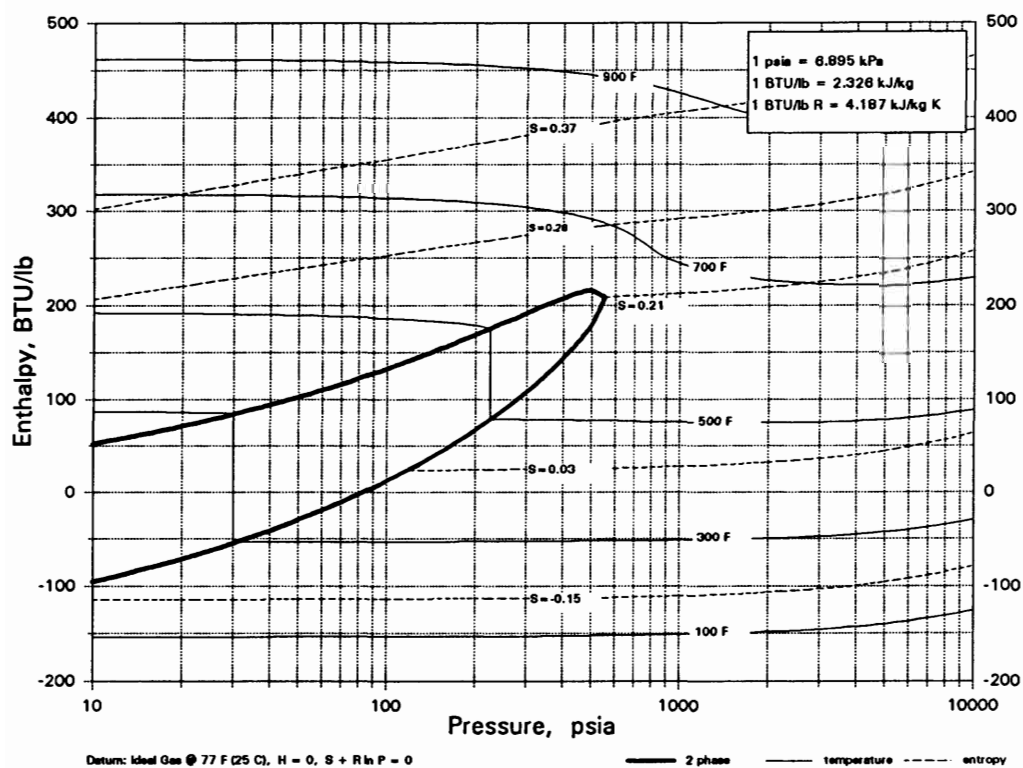
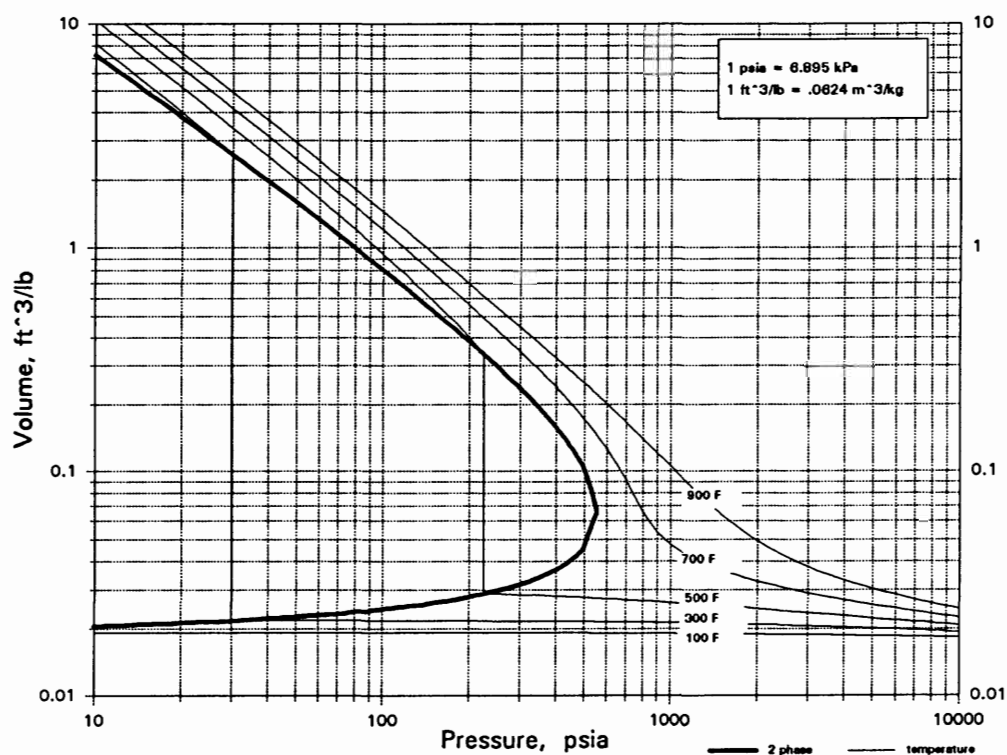
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DIETHYL MALONATE

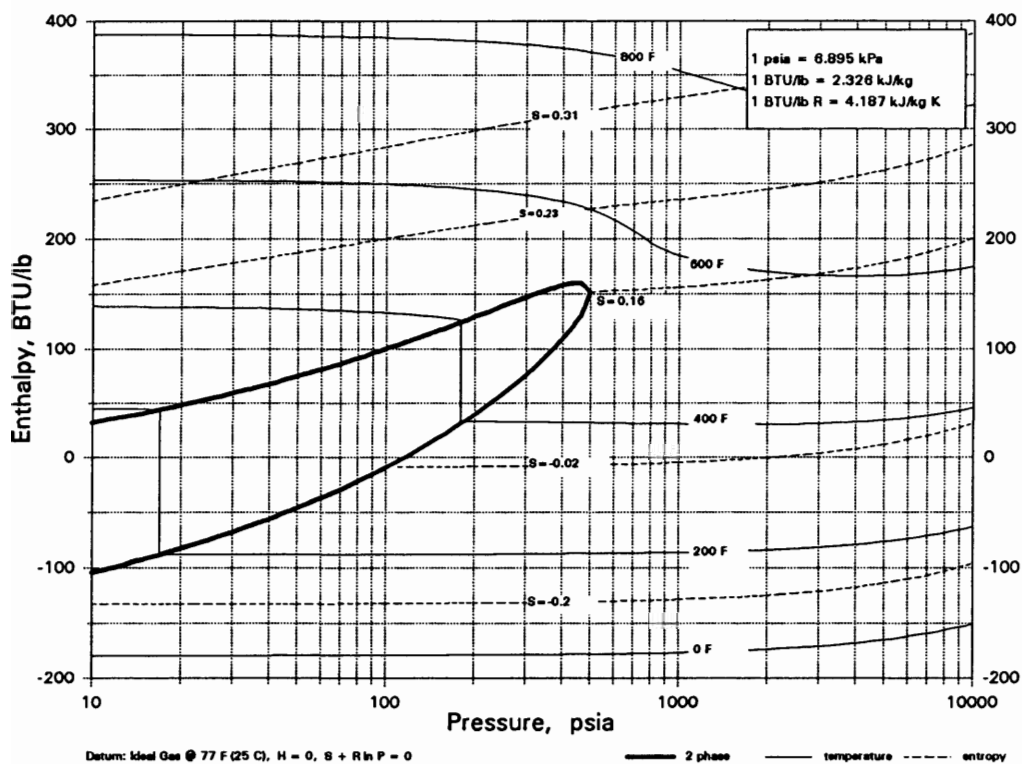
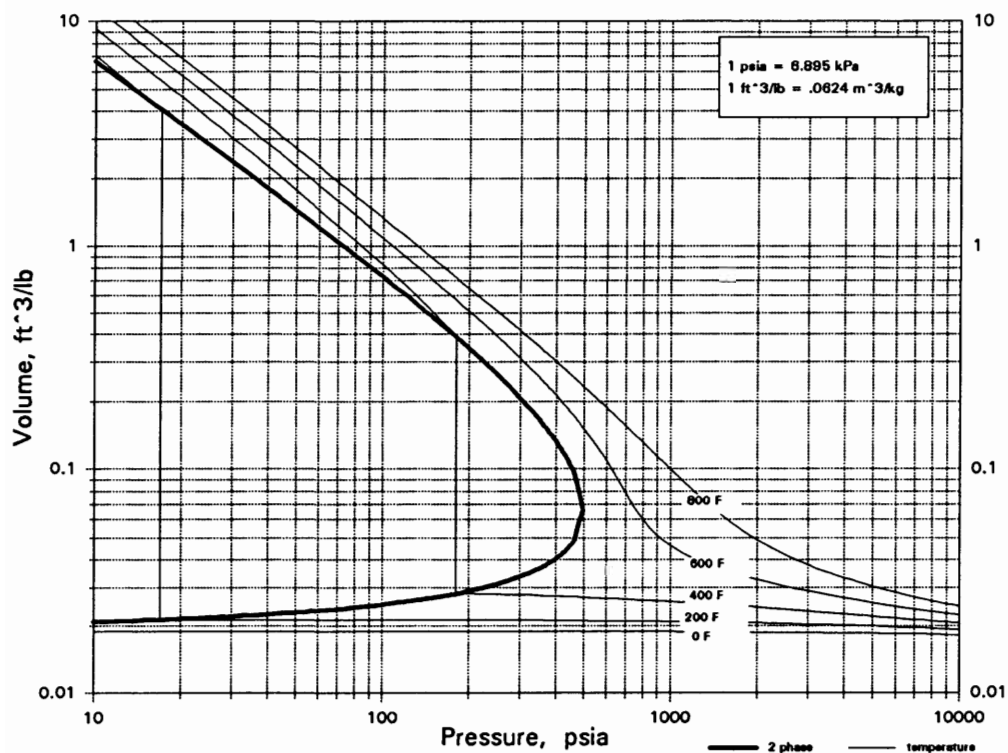


C7H14

CYCLOHEPTANE

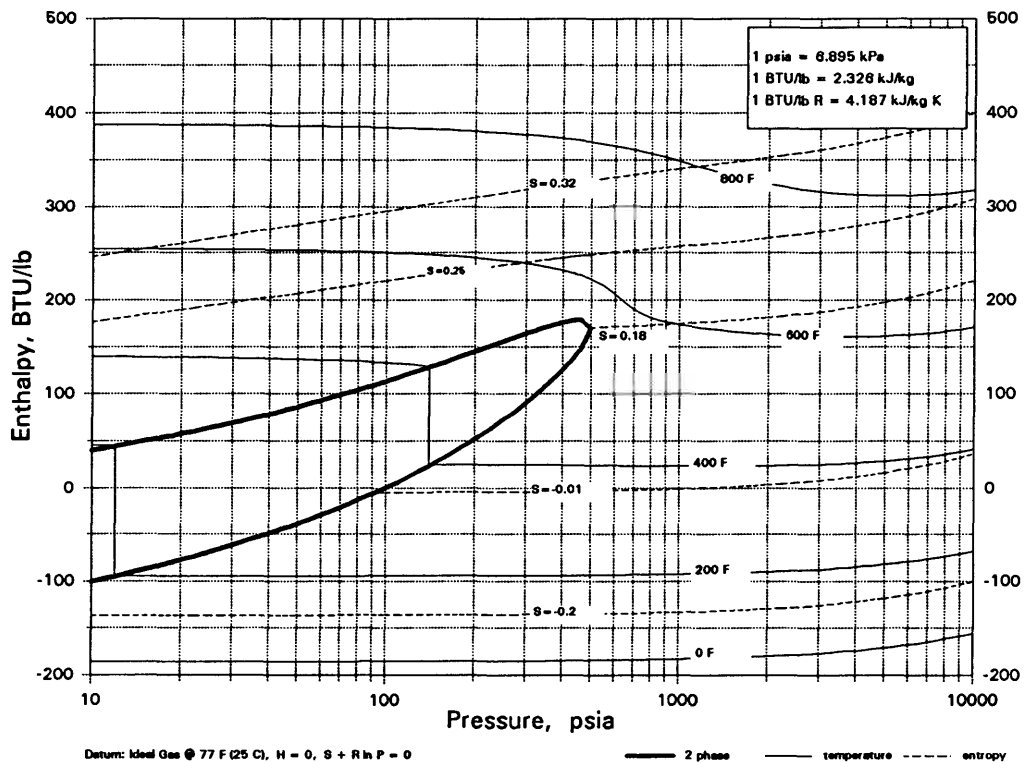
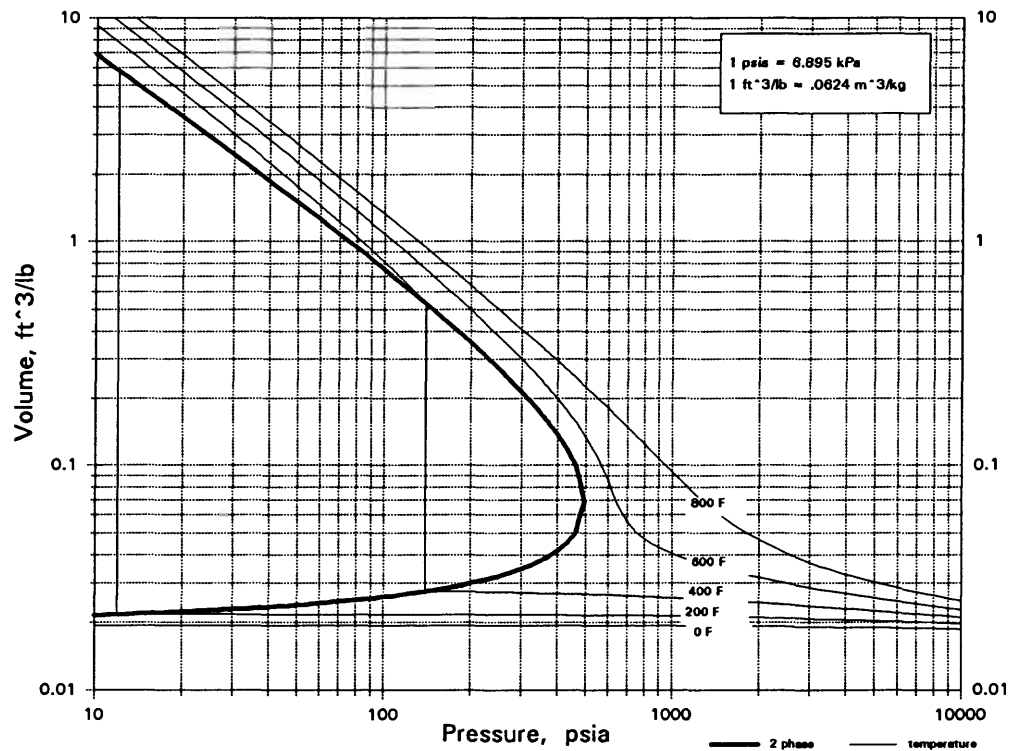


C7H14
1-1-DIMETHYLCYCLOPENTANE



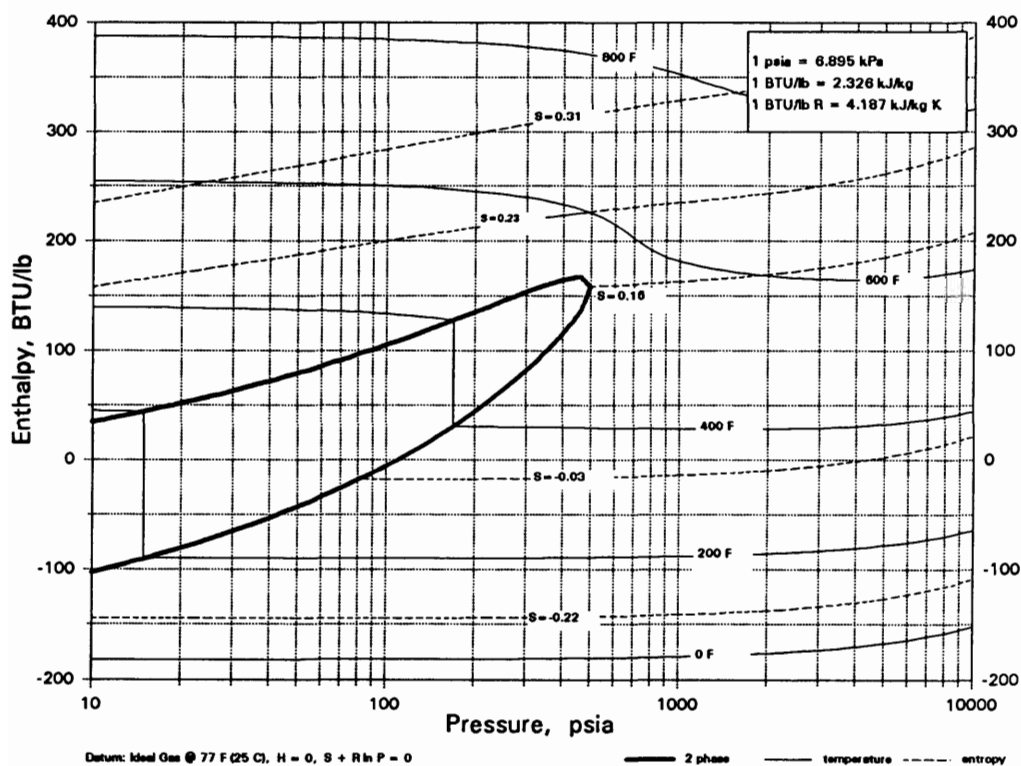
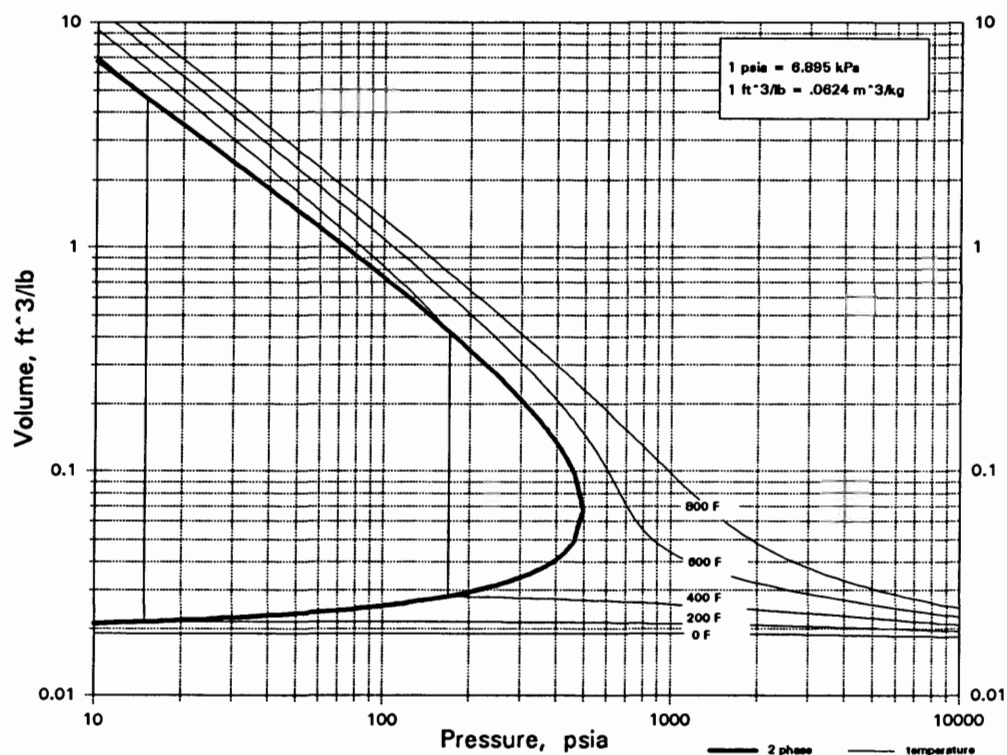
C7H14

cis-1-2-DIMETHYLCYCLOPENTANE



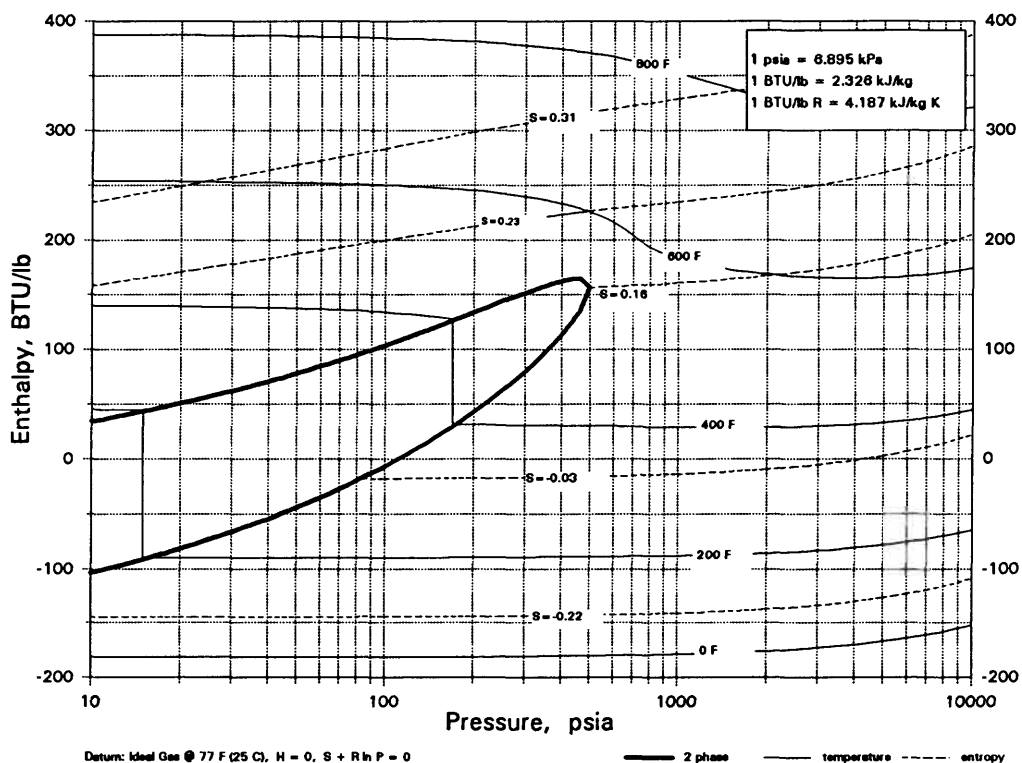
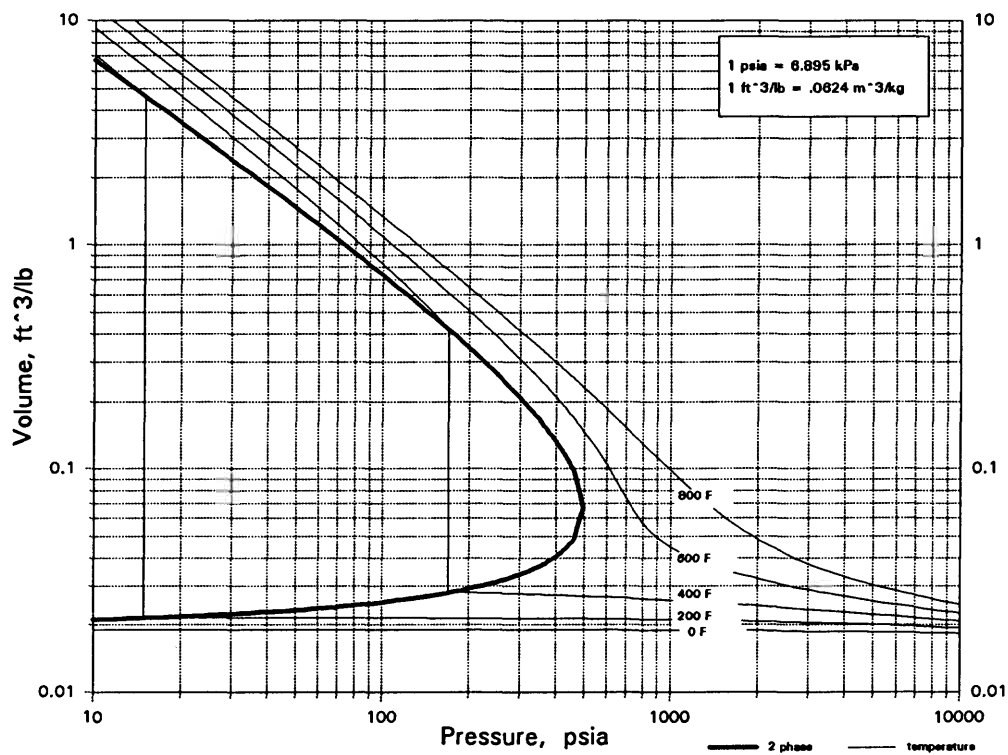
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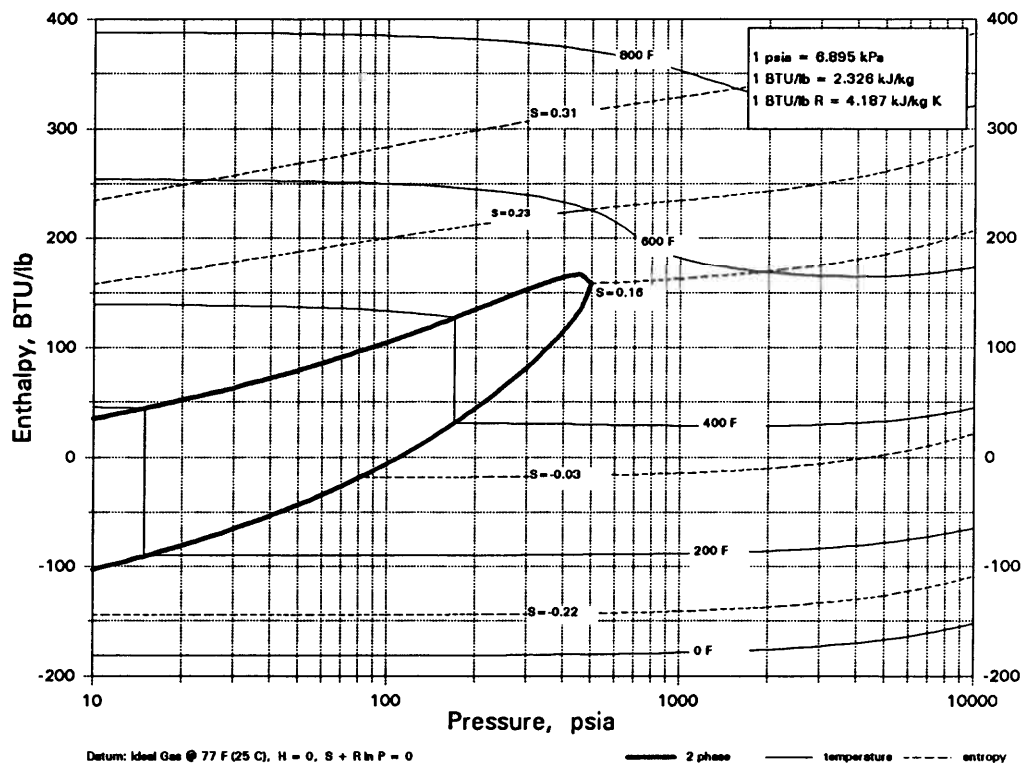
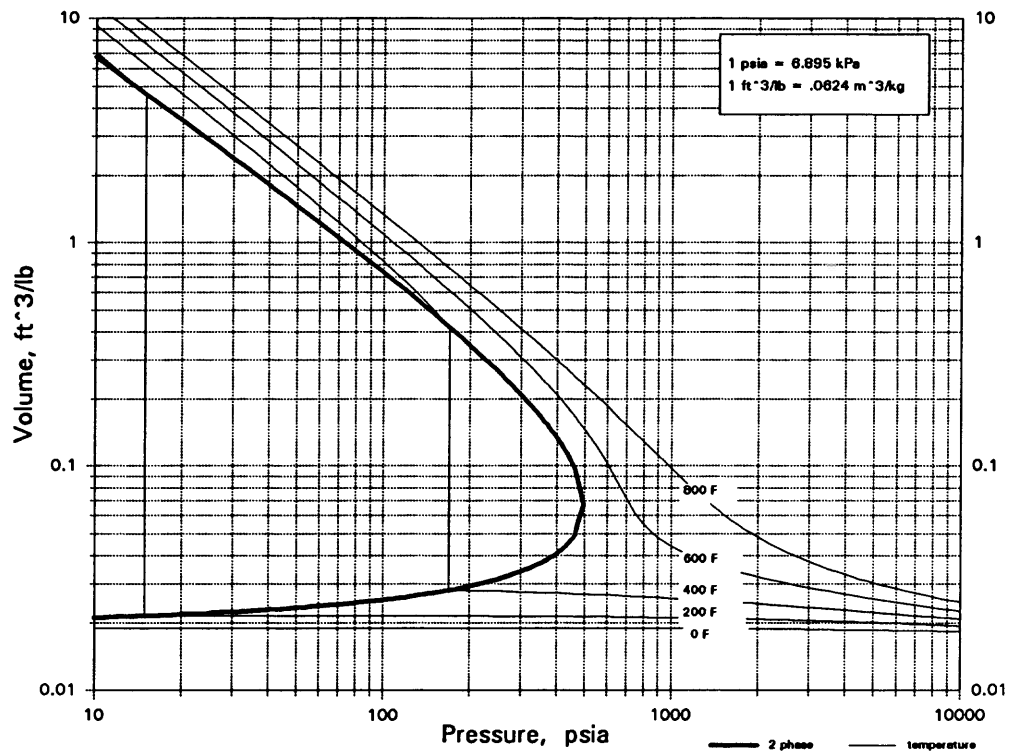
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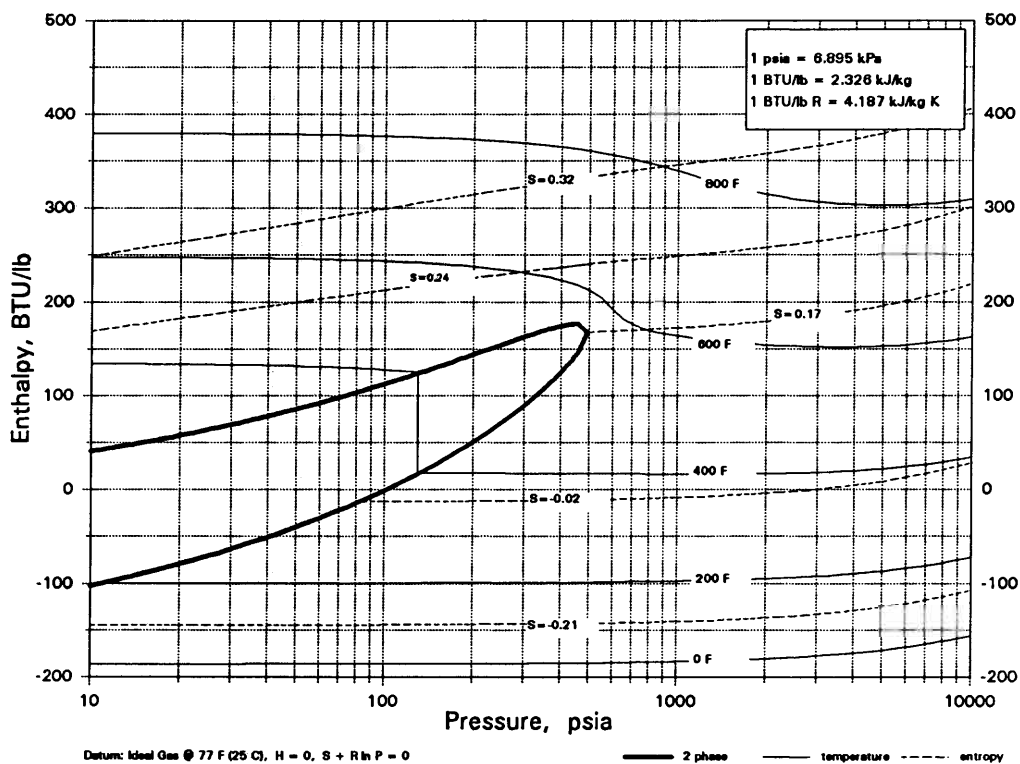
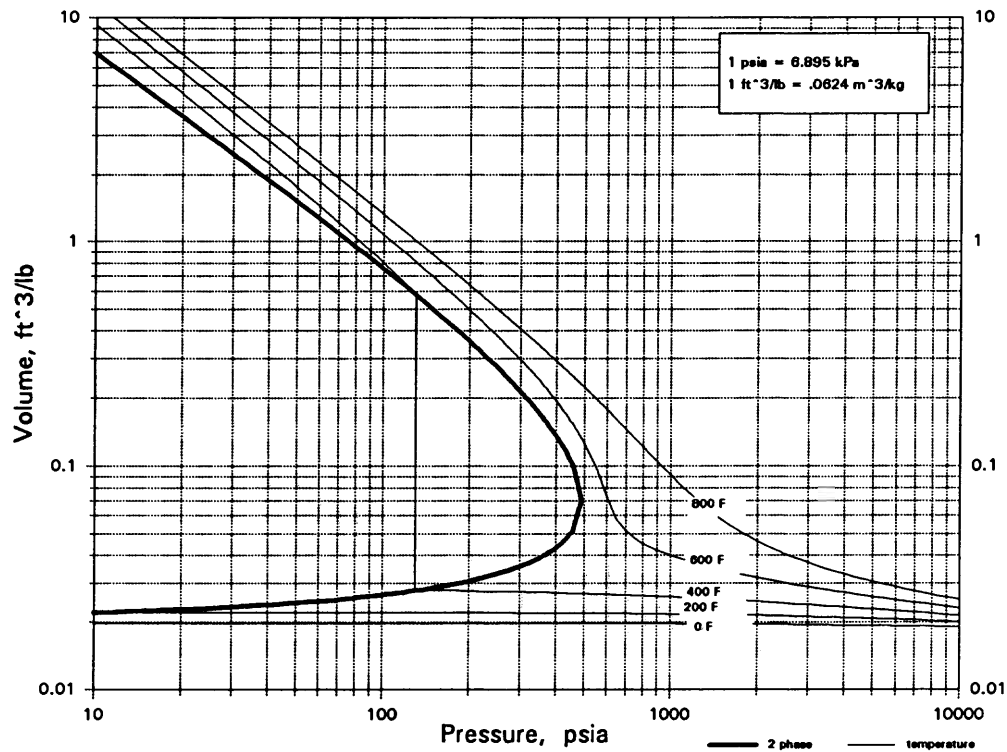
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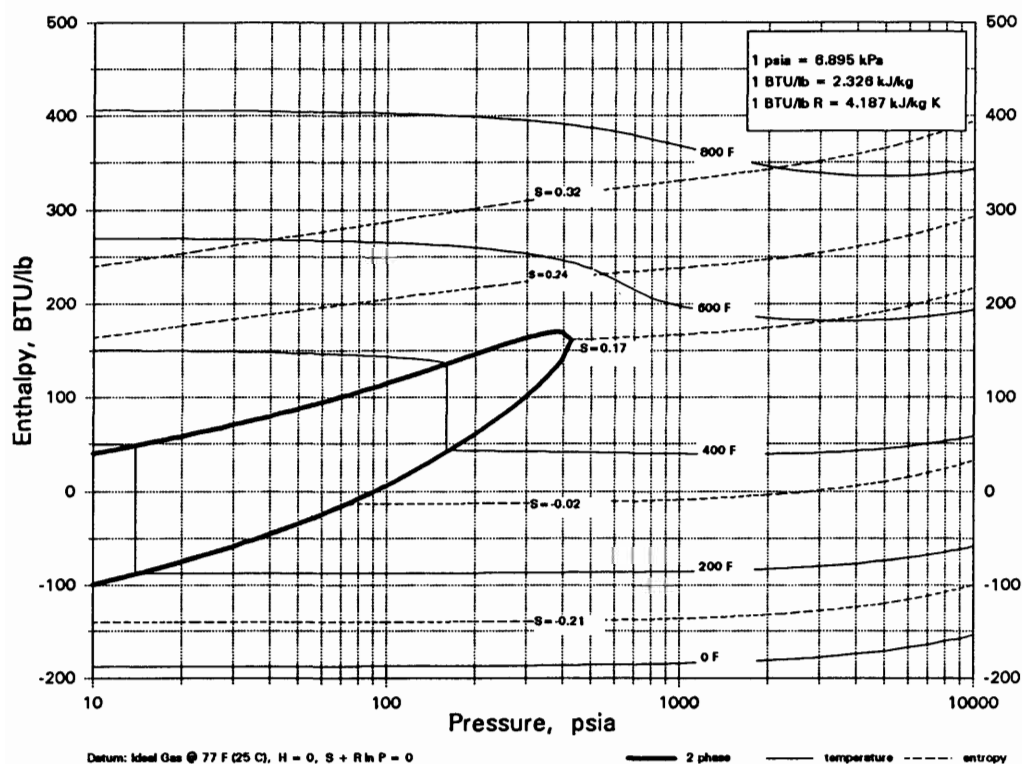
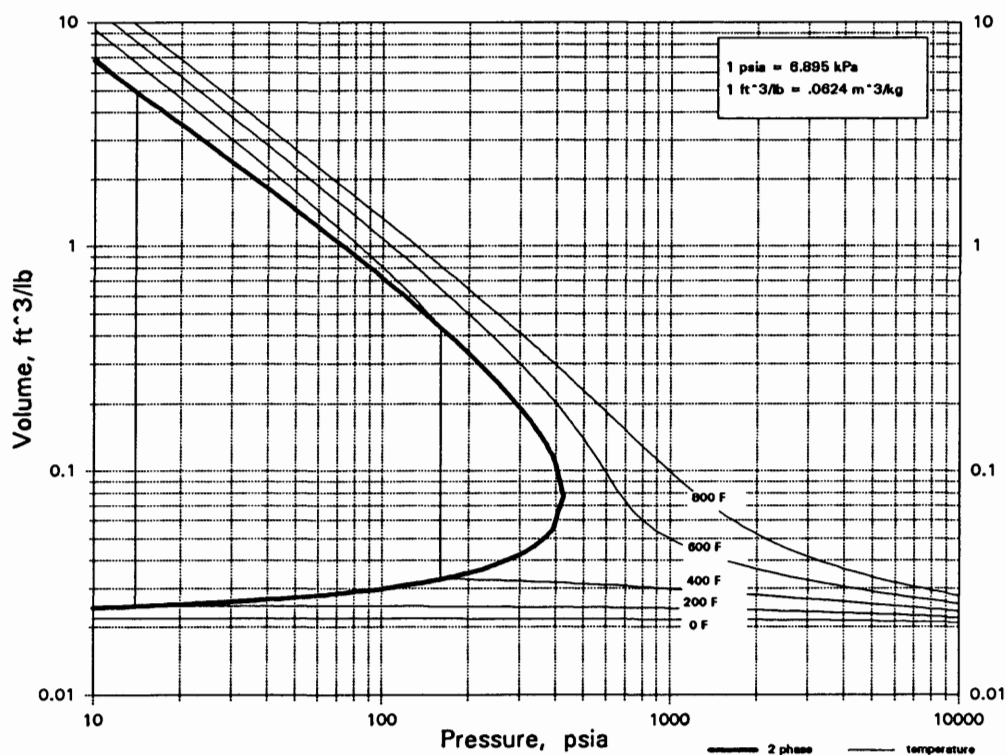
C7H14

ETHYLCYCLOPENTANE



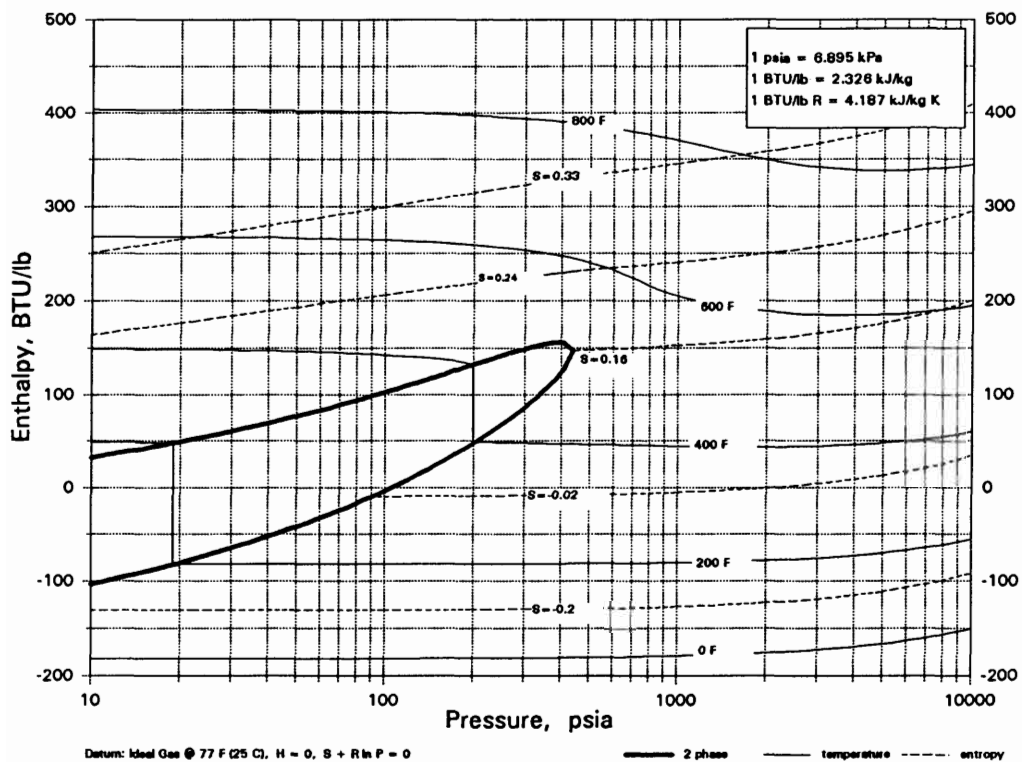
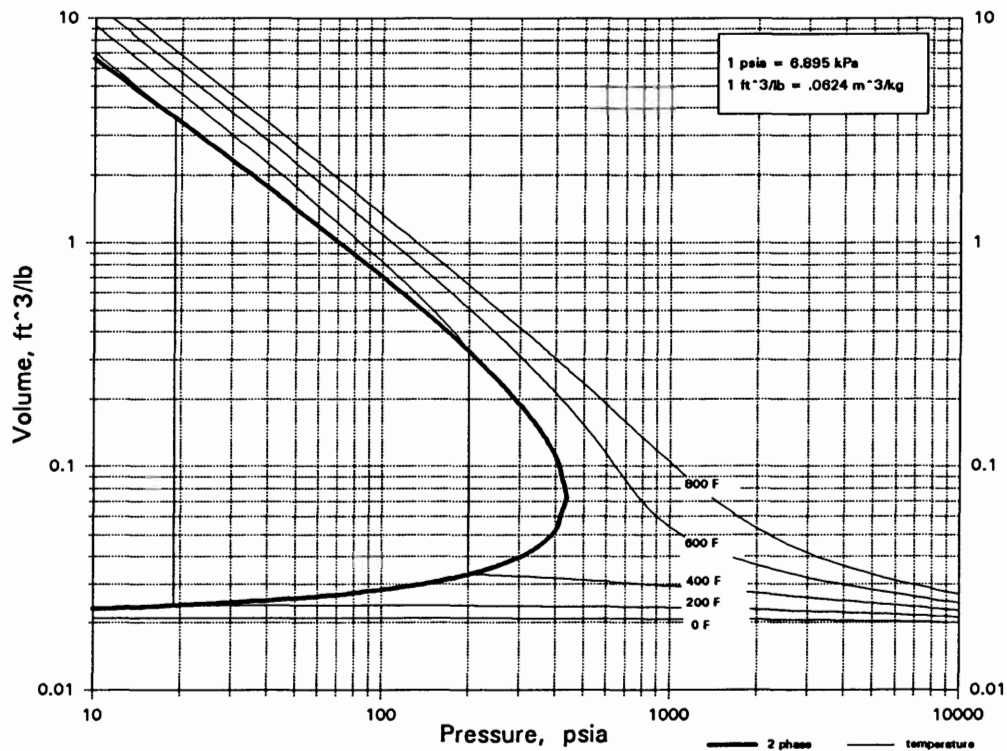
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2-ETHYL-1-PENTENE



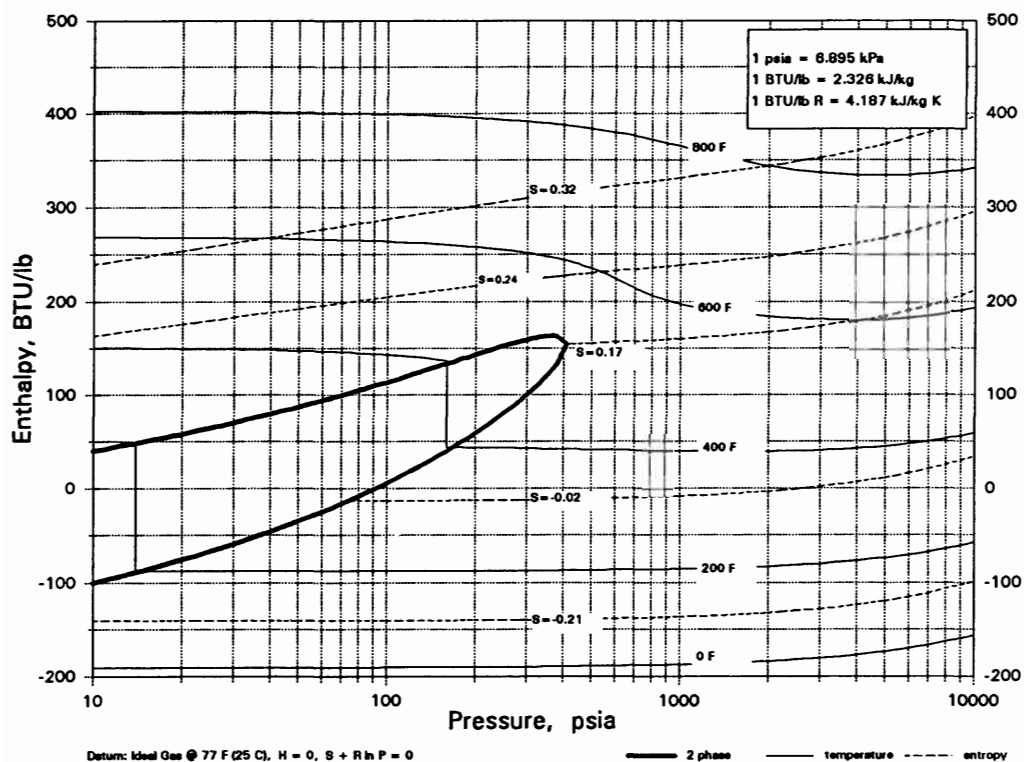
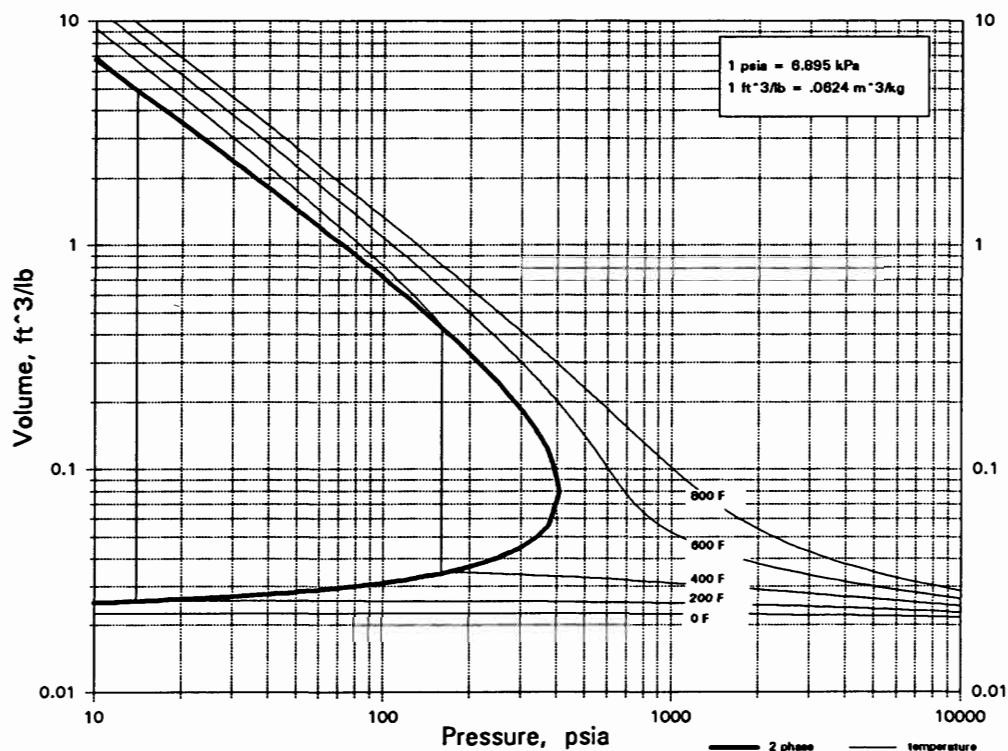
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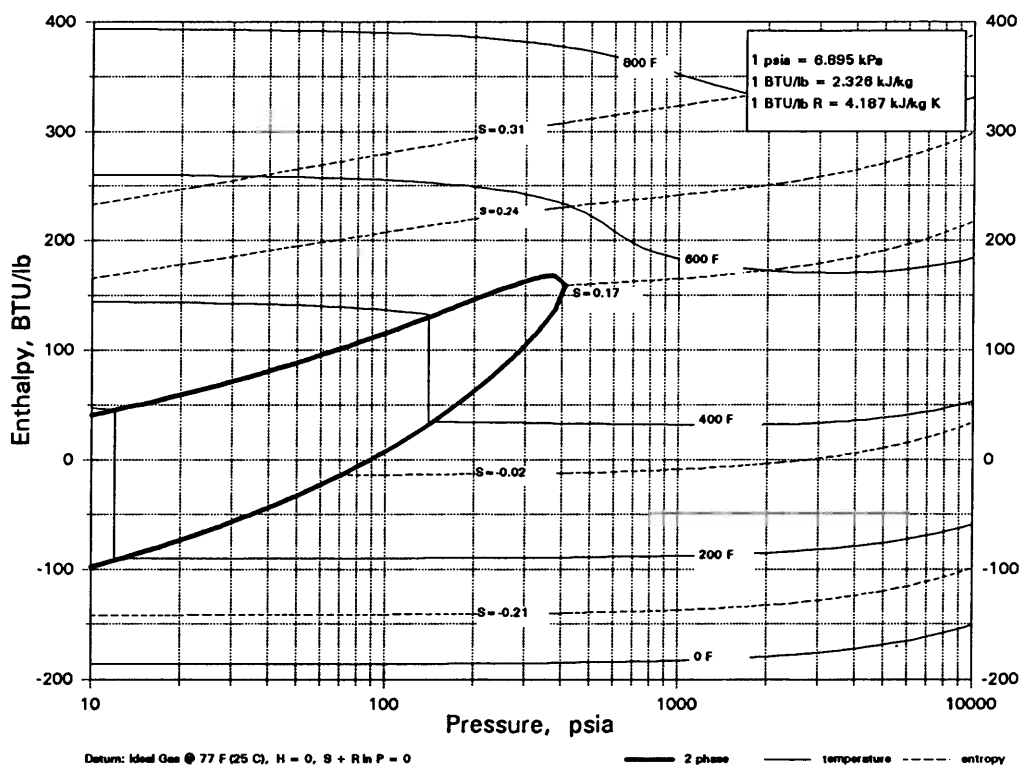
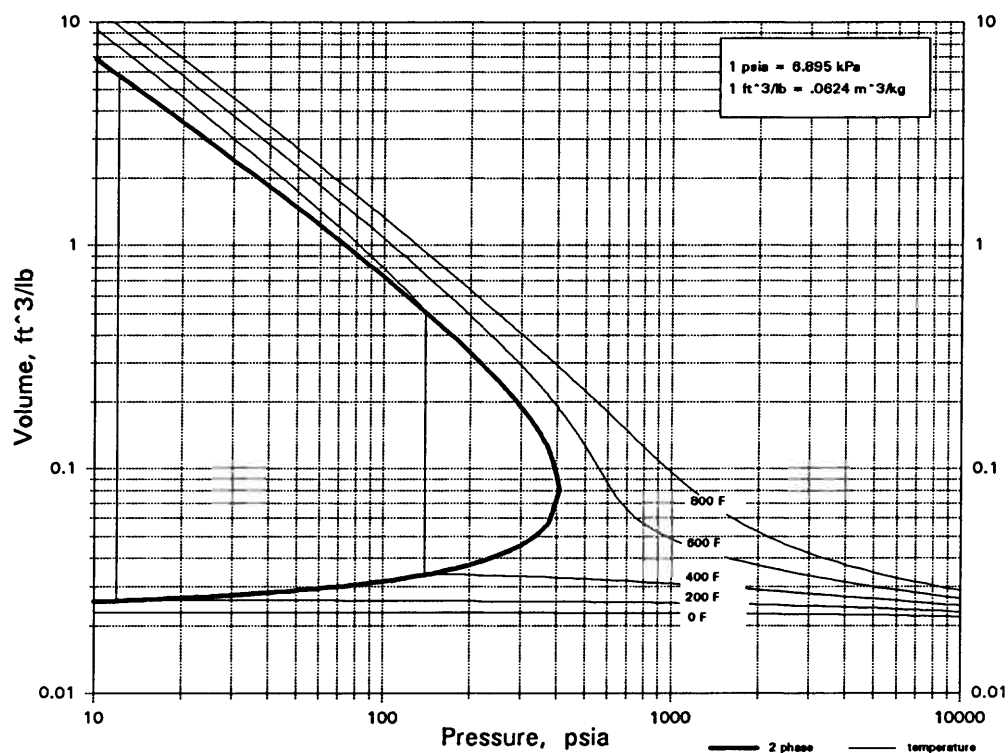
C7H14

1-HEPTENE



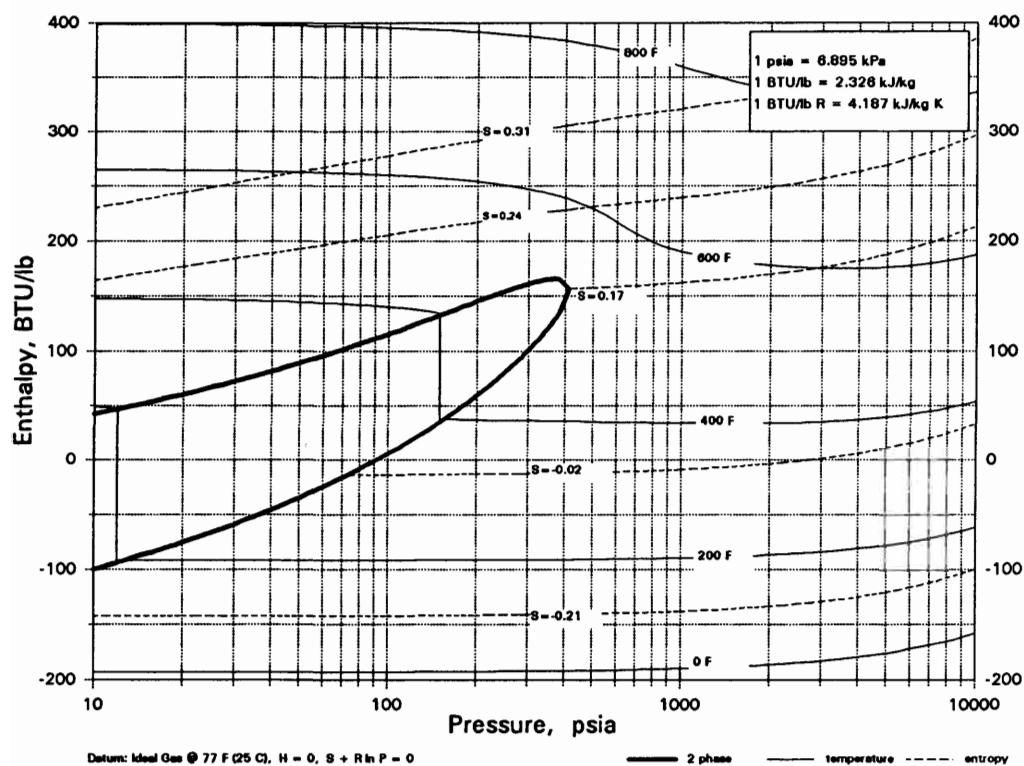
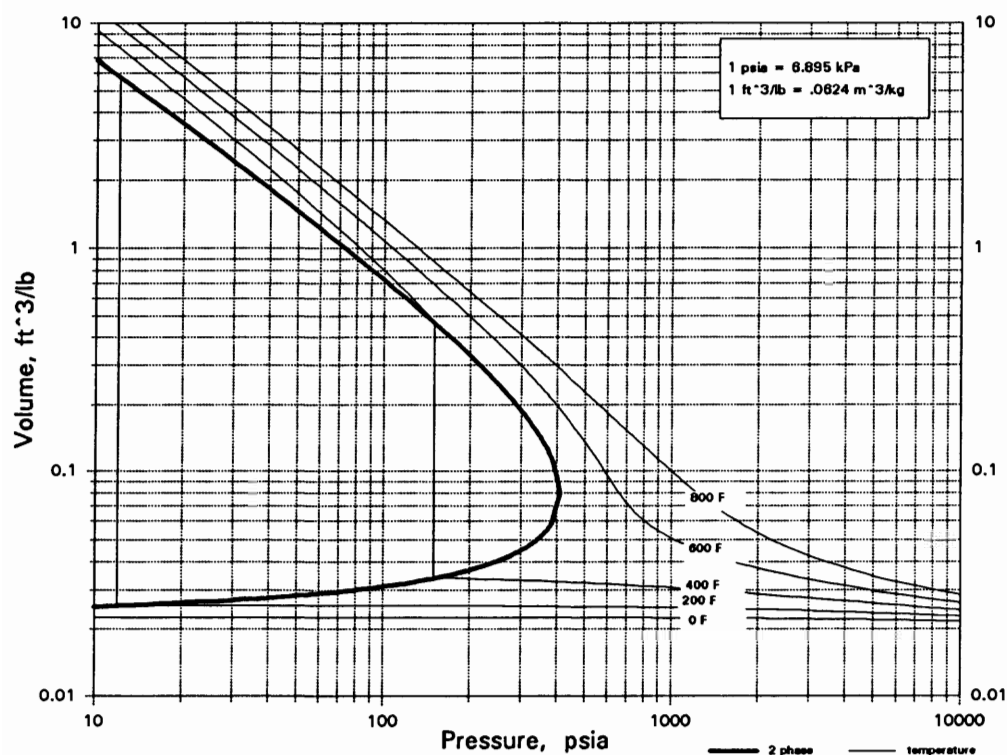
C7H14

cis-2-HEPTENE



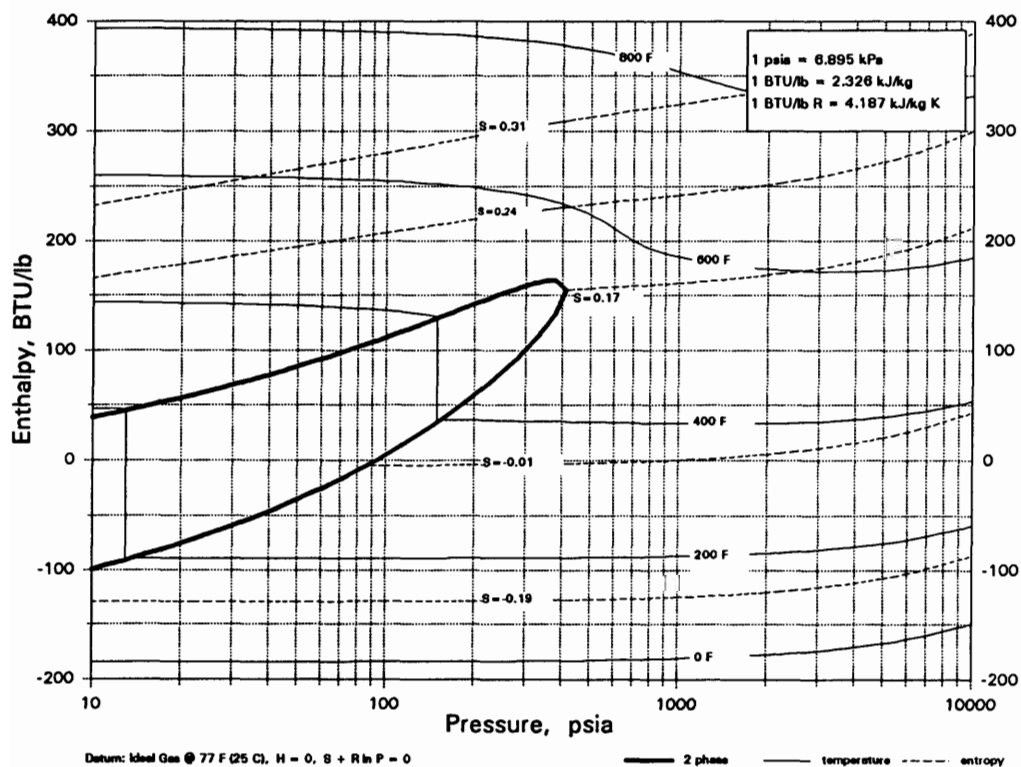
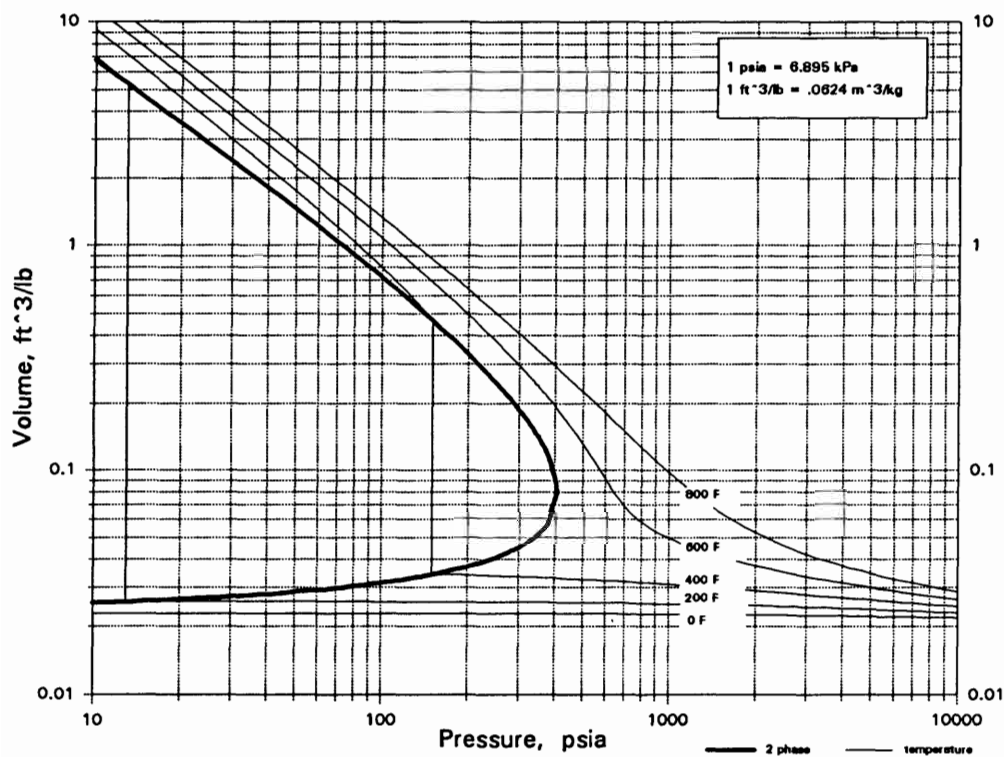
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trans-2-HEPTENE



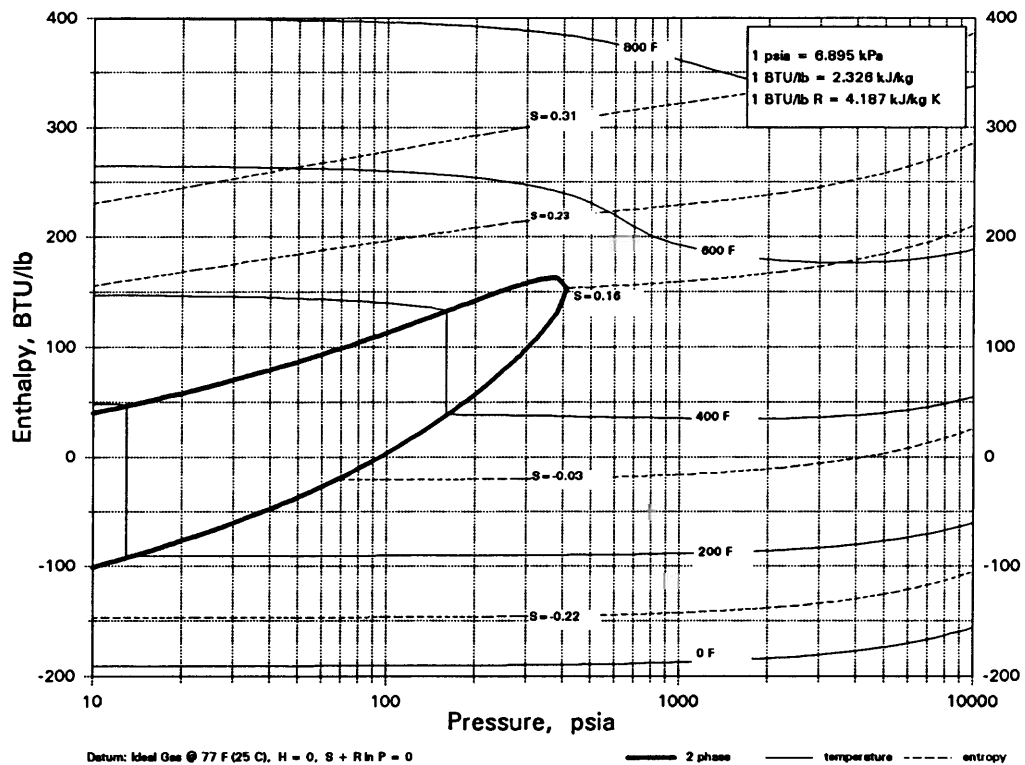
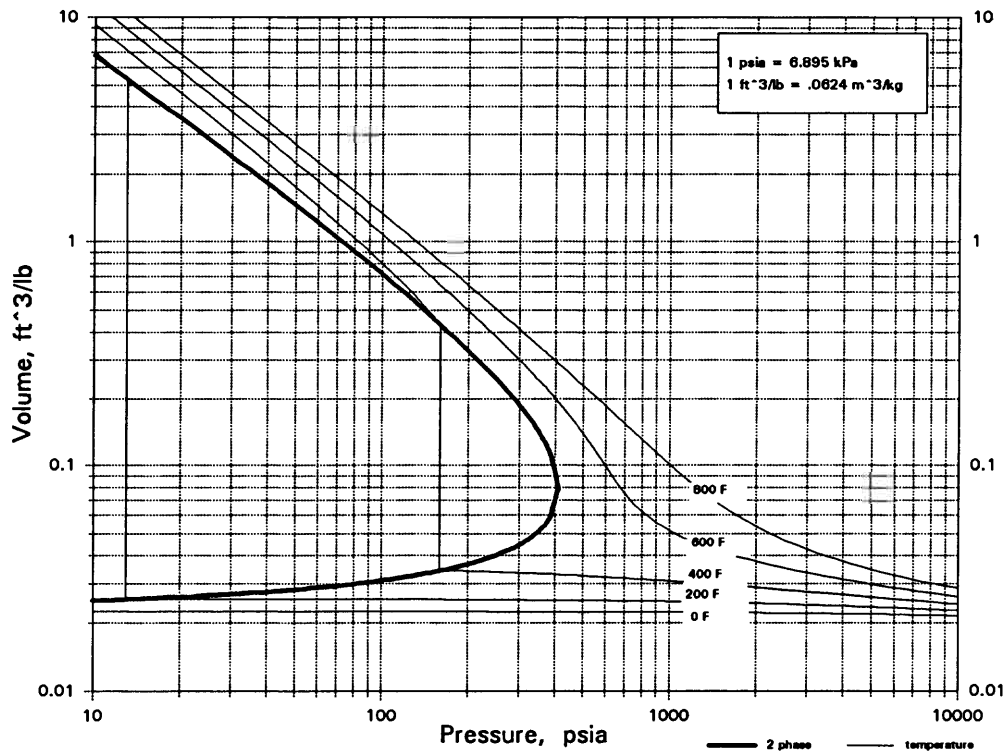
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cis-3-HEPTENE



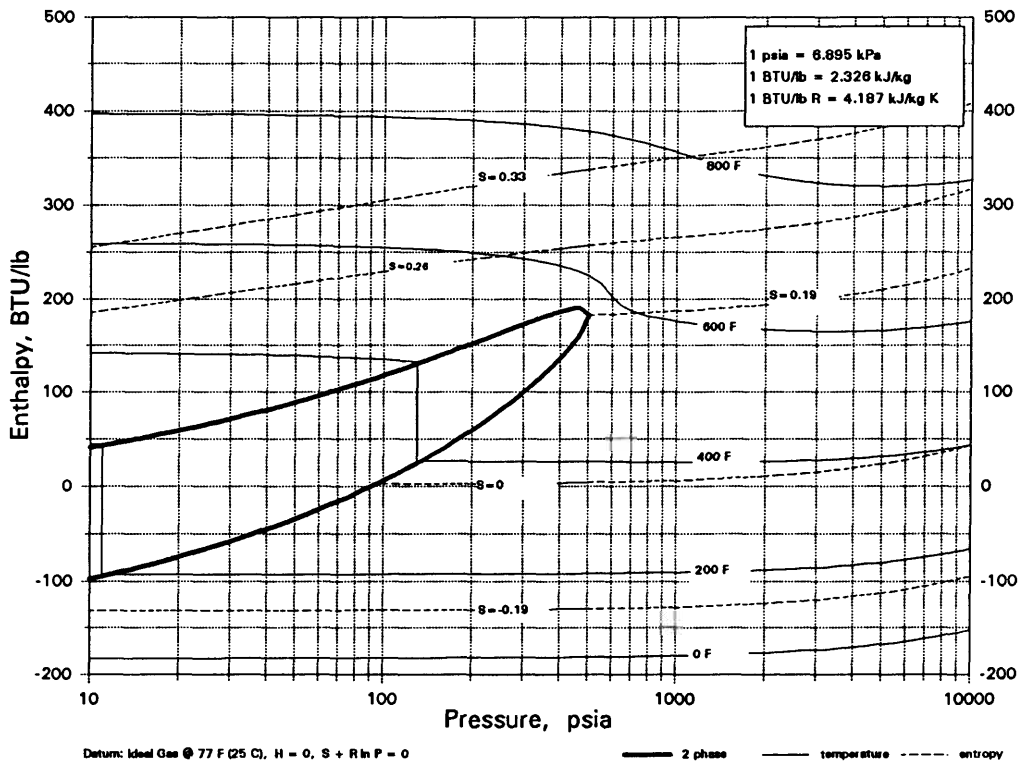
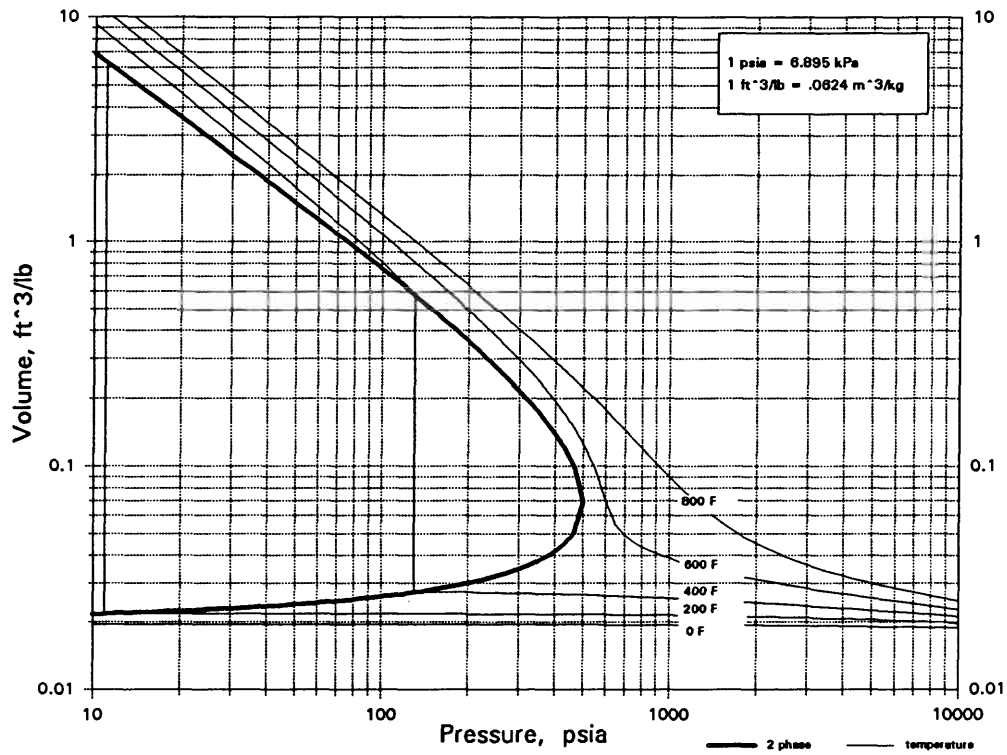
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trans-3-HEPTENE



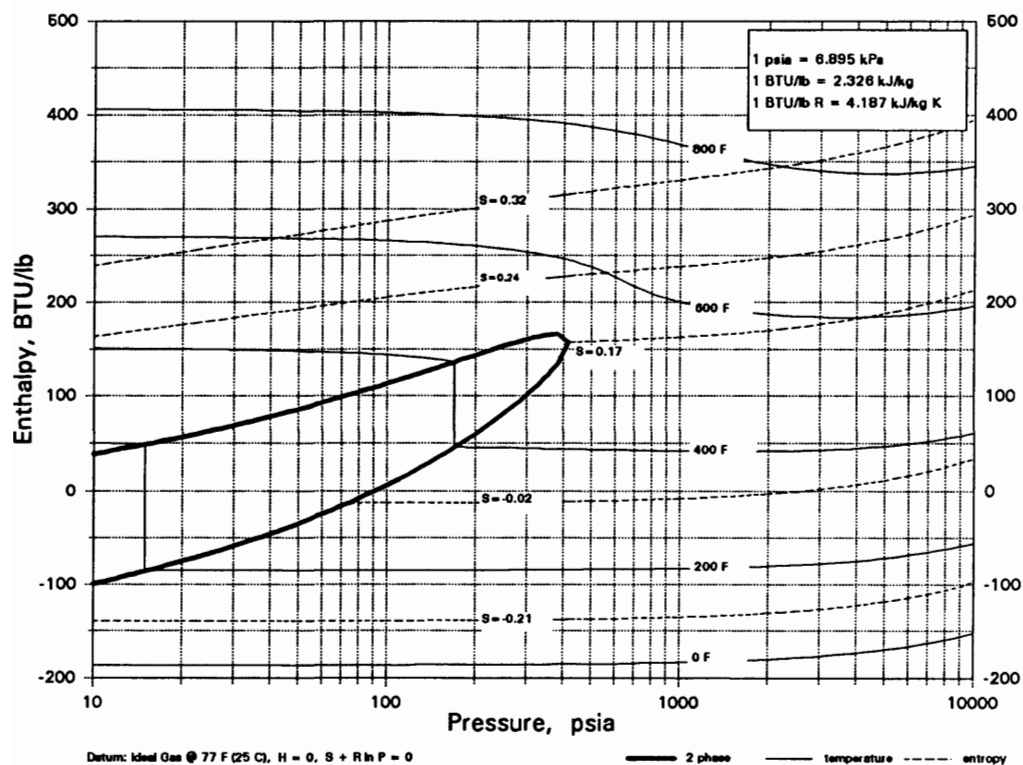
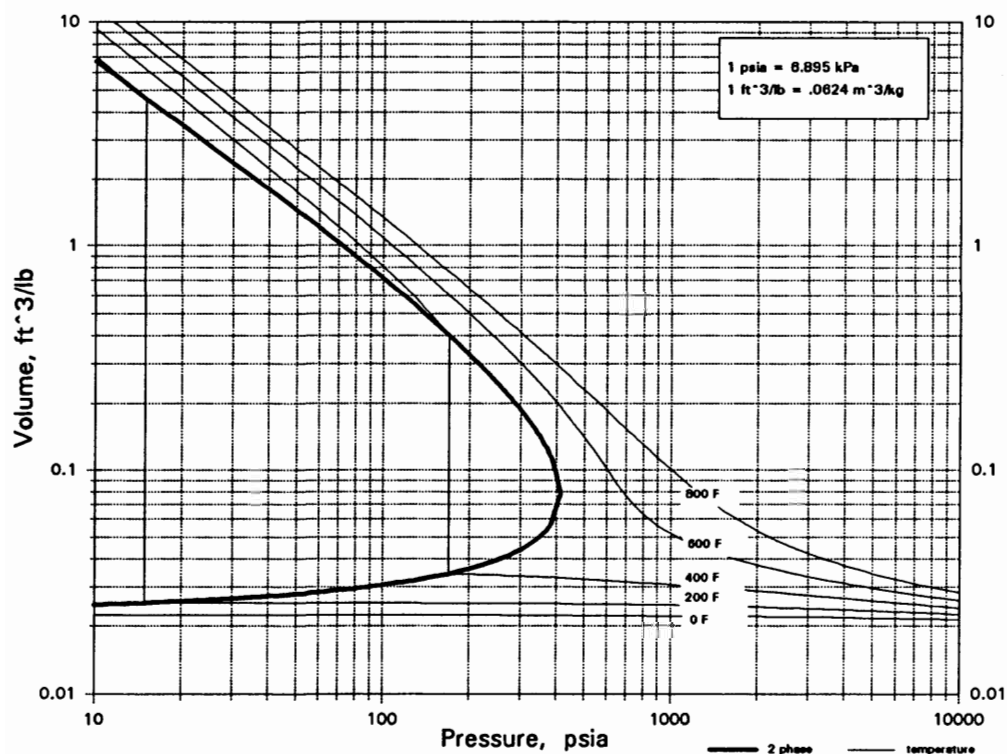
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METHYLCYCLOHEXANE



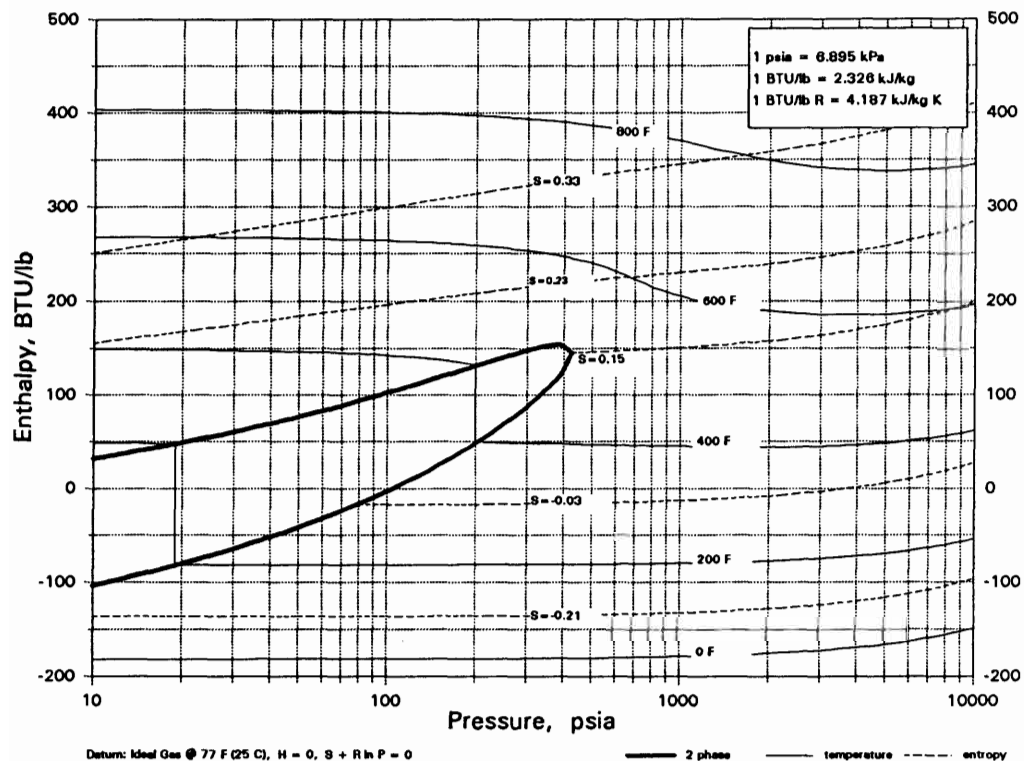
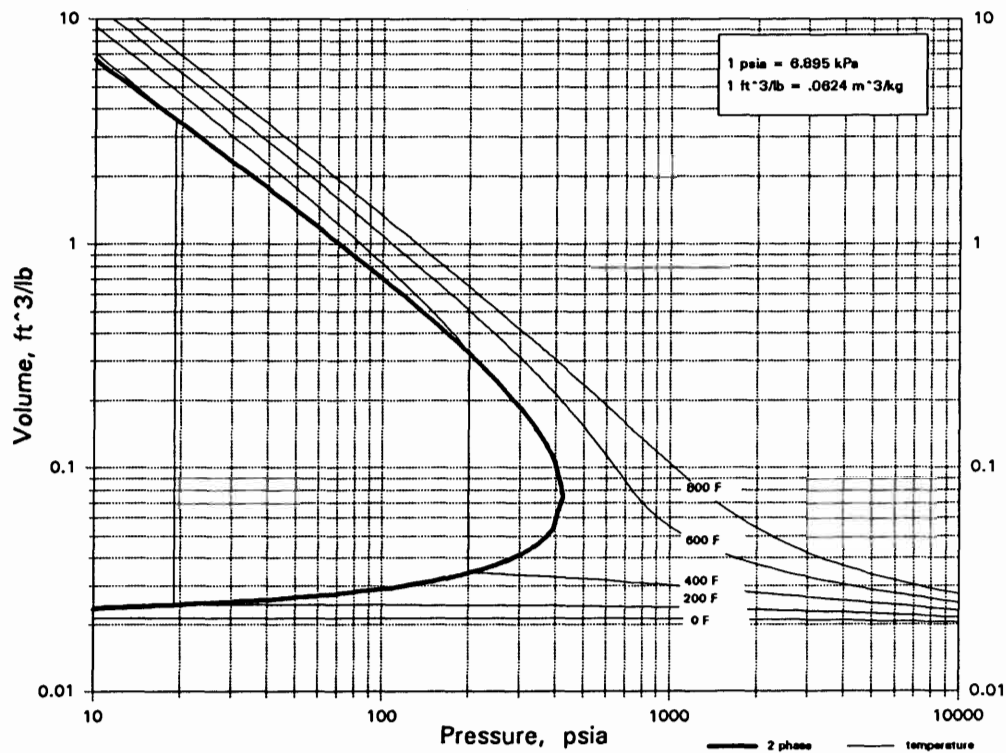
C7H14

2-METHYL-1-HEXENE

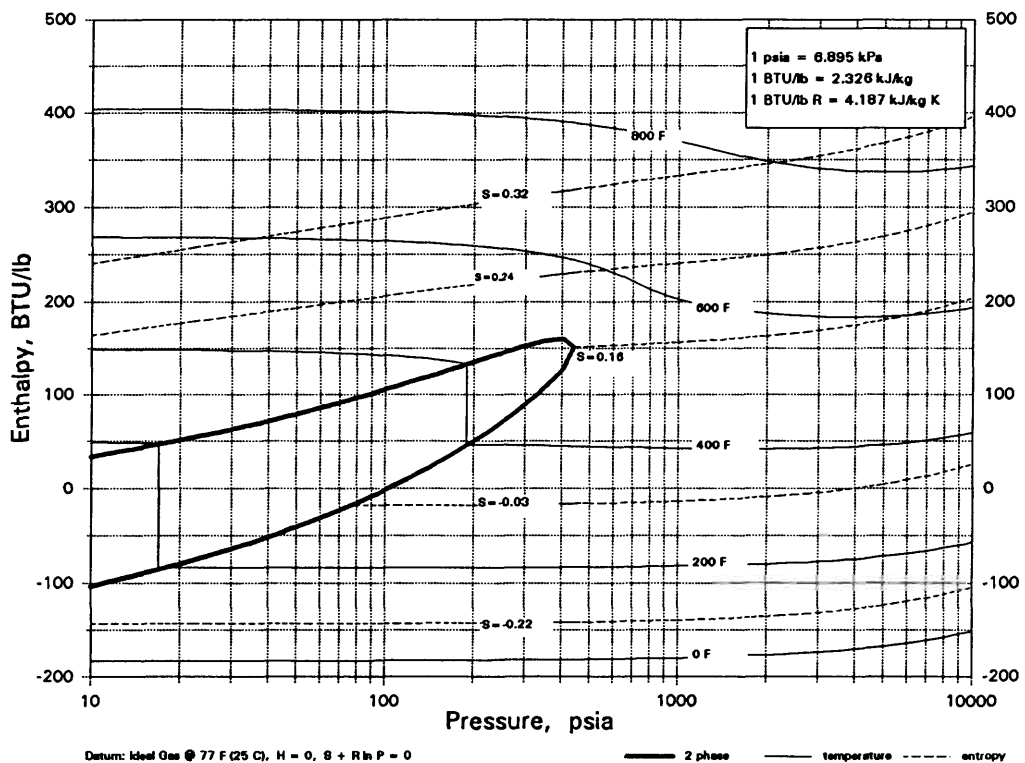
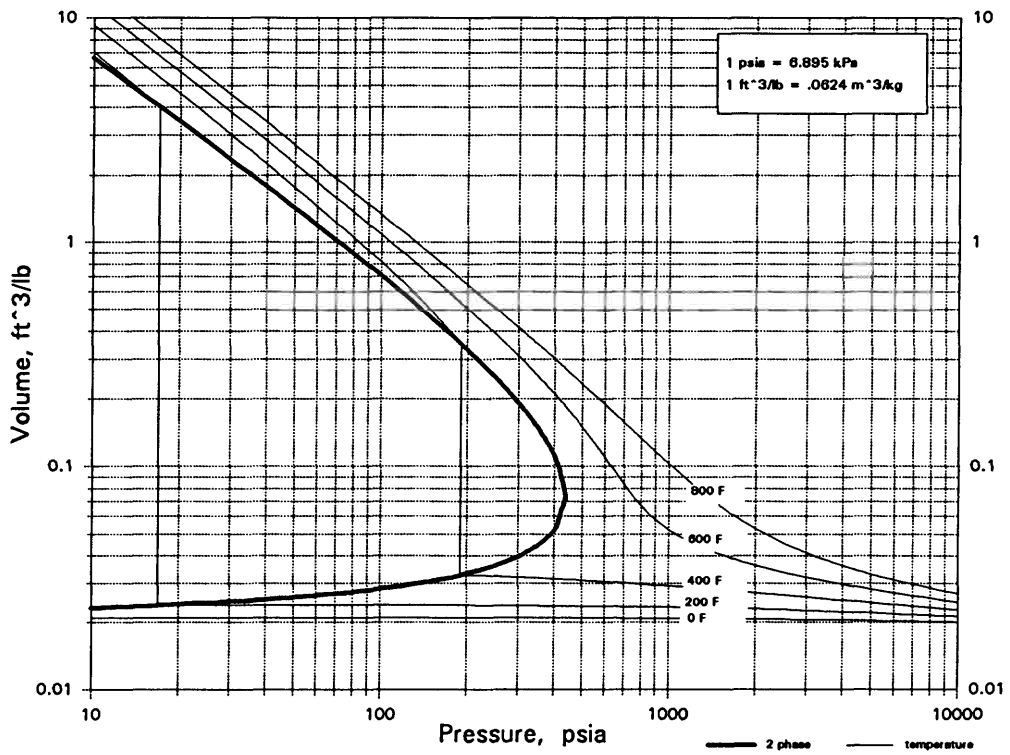


C7H14

3-METHYL-1-HEXENE

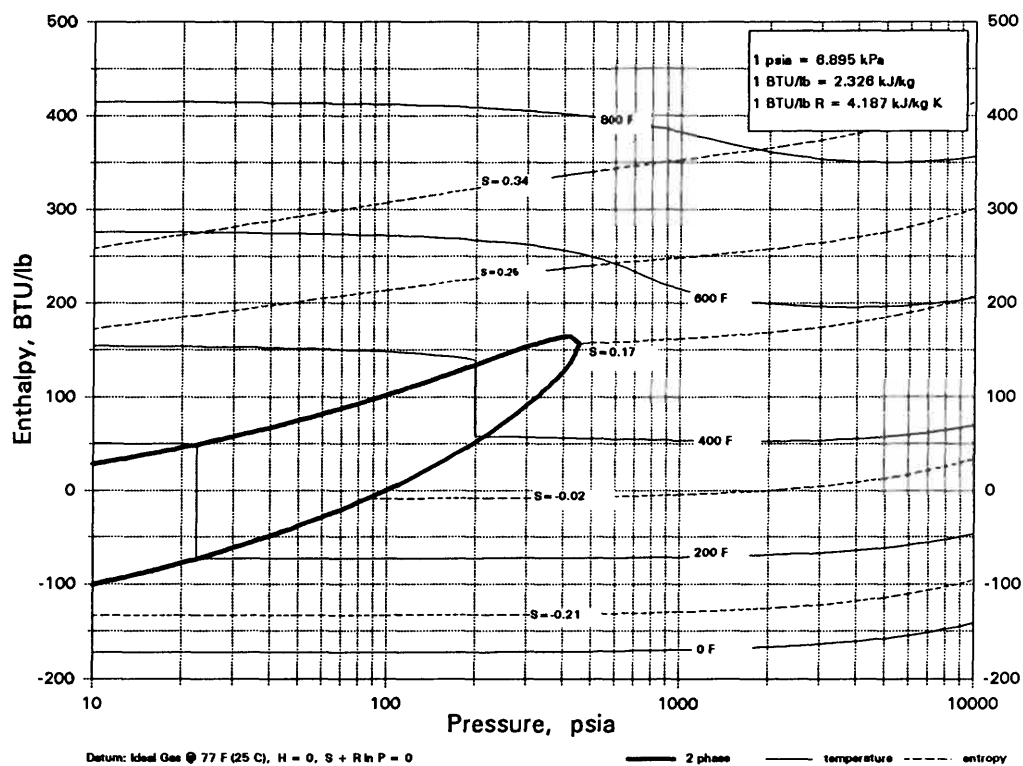
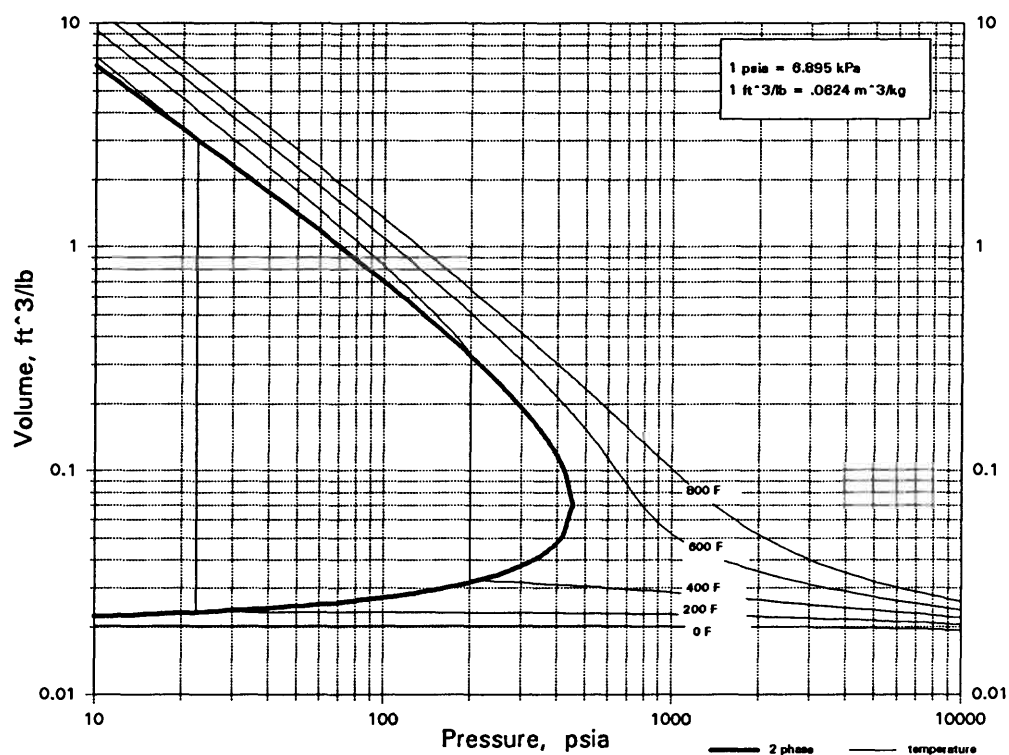


C7H14
4-METHYL-1-HEXENE



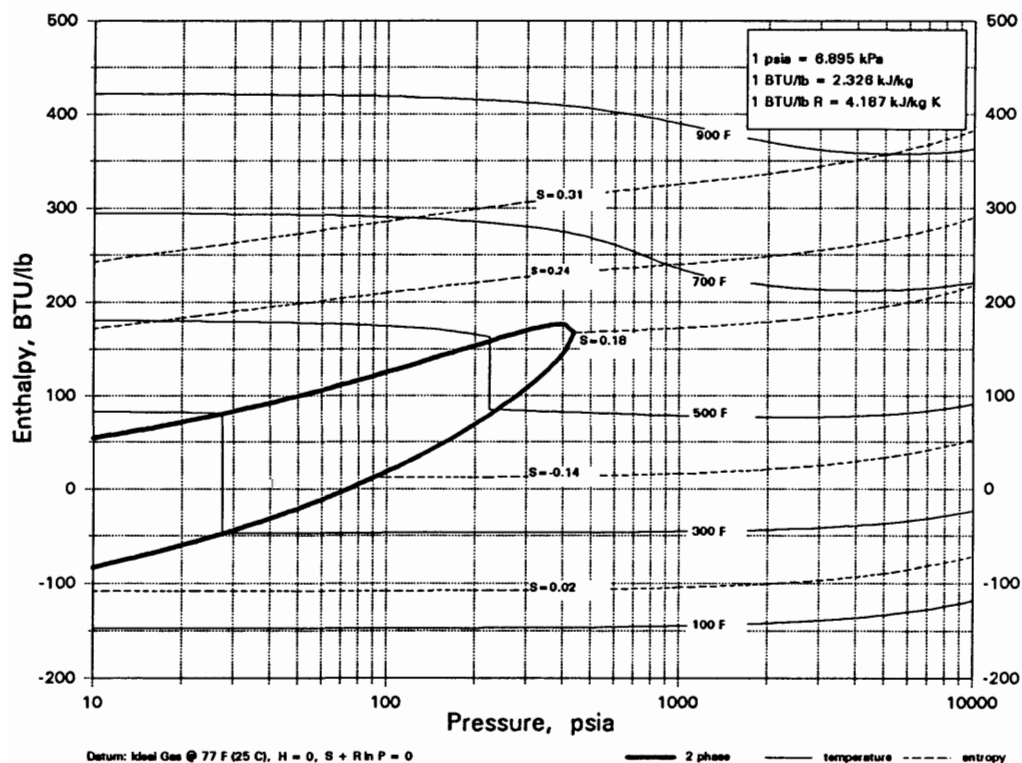
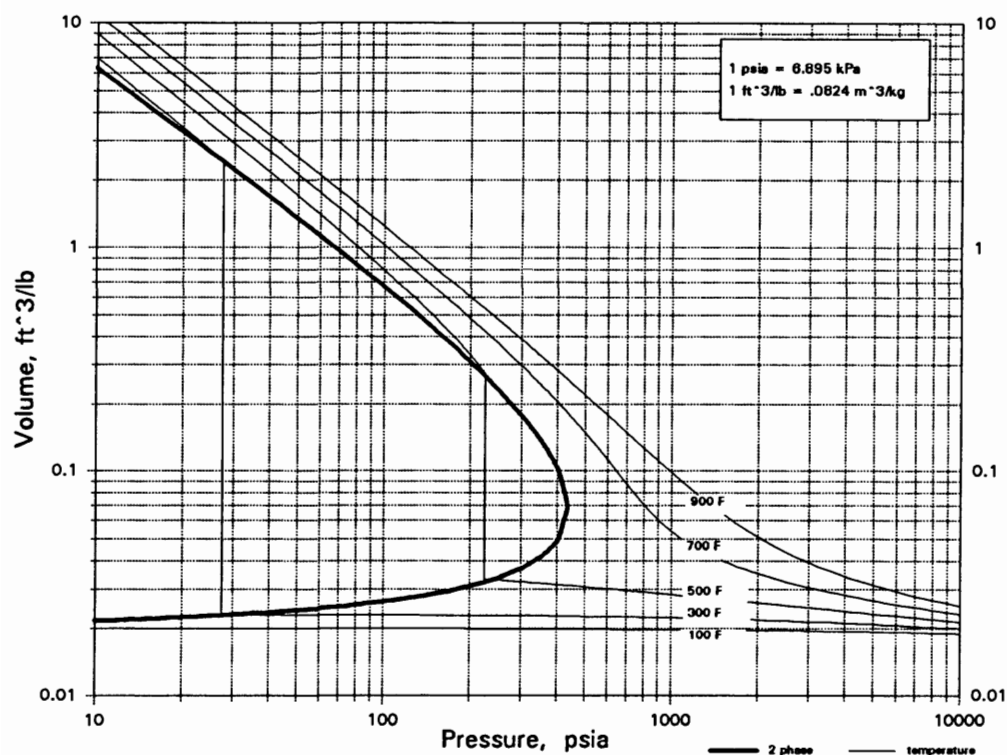
C7H14

2-3-3-TRIMETHYL-1-BUTENE



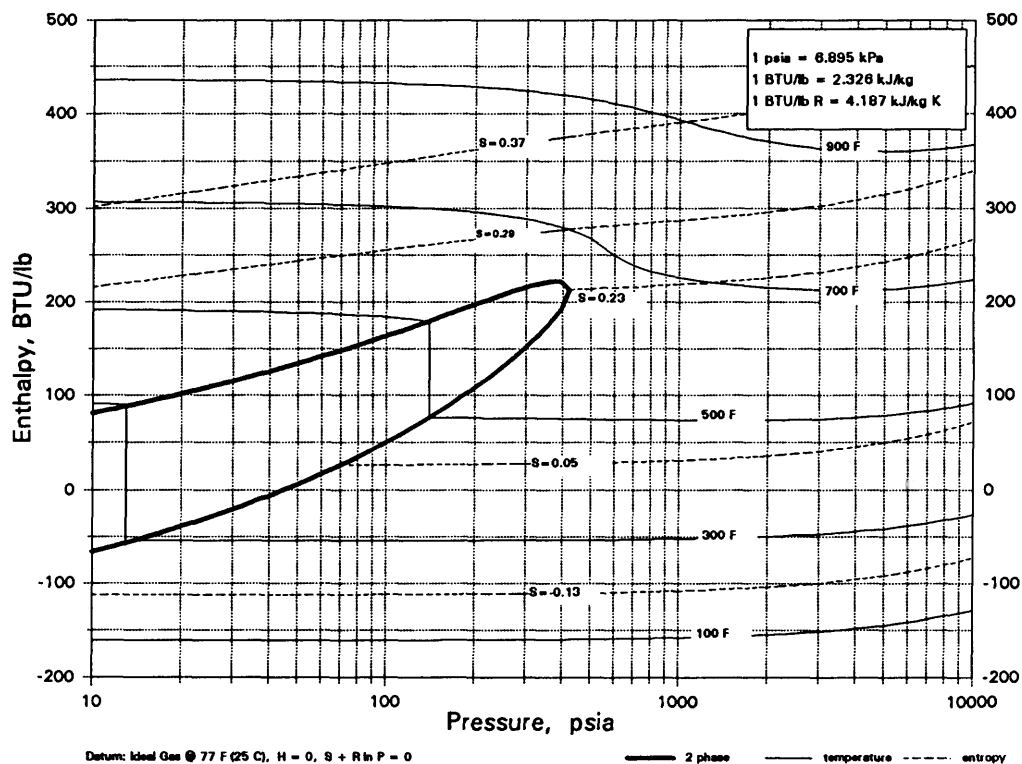
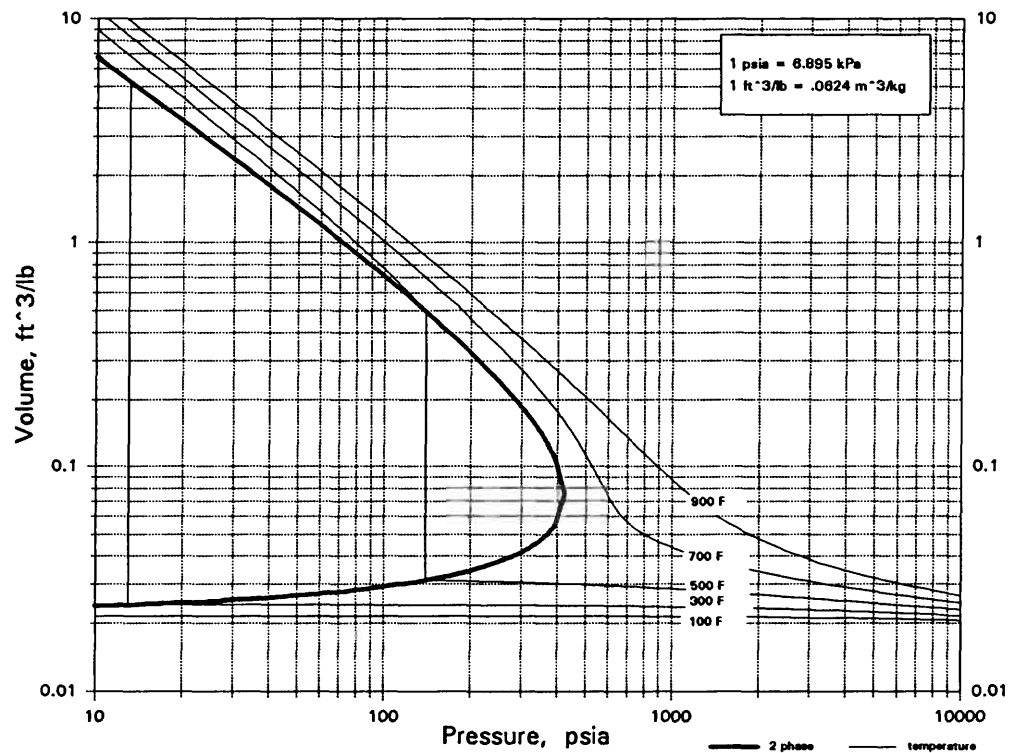
C7H14O

DIISOPROPYL KETONE

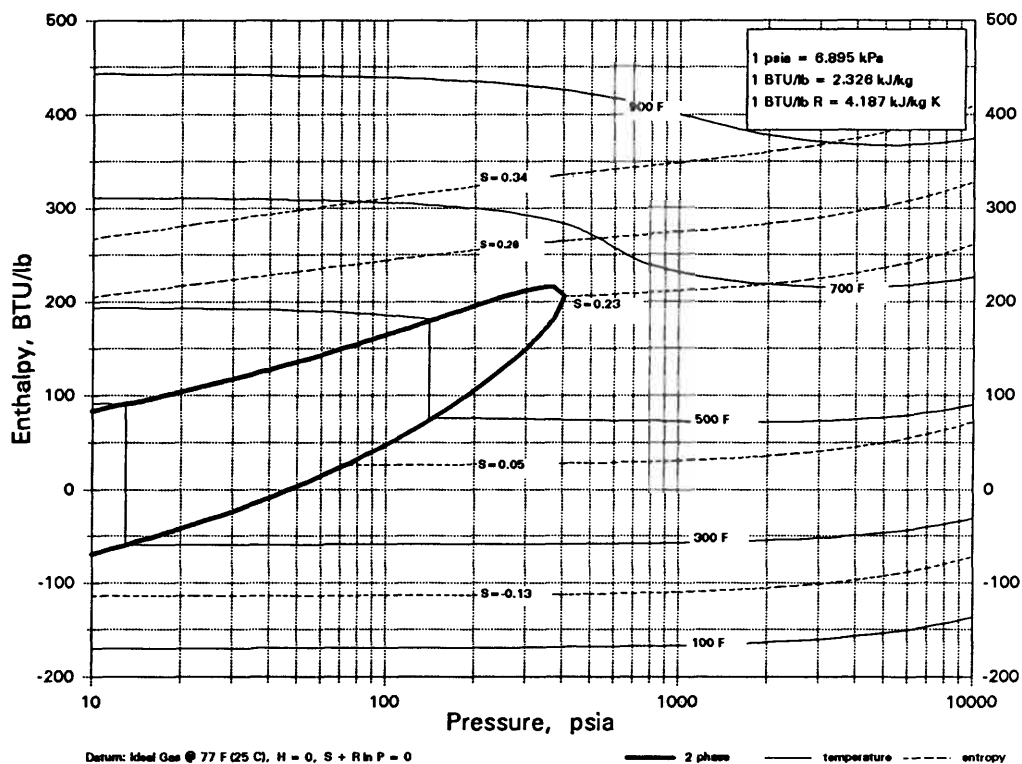
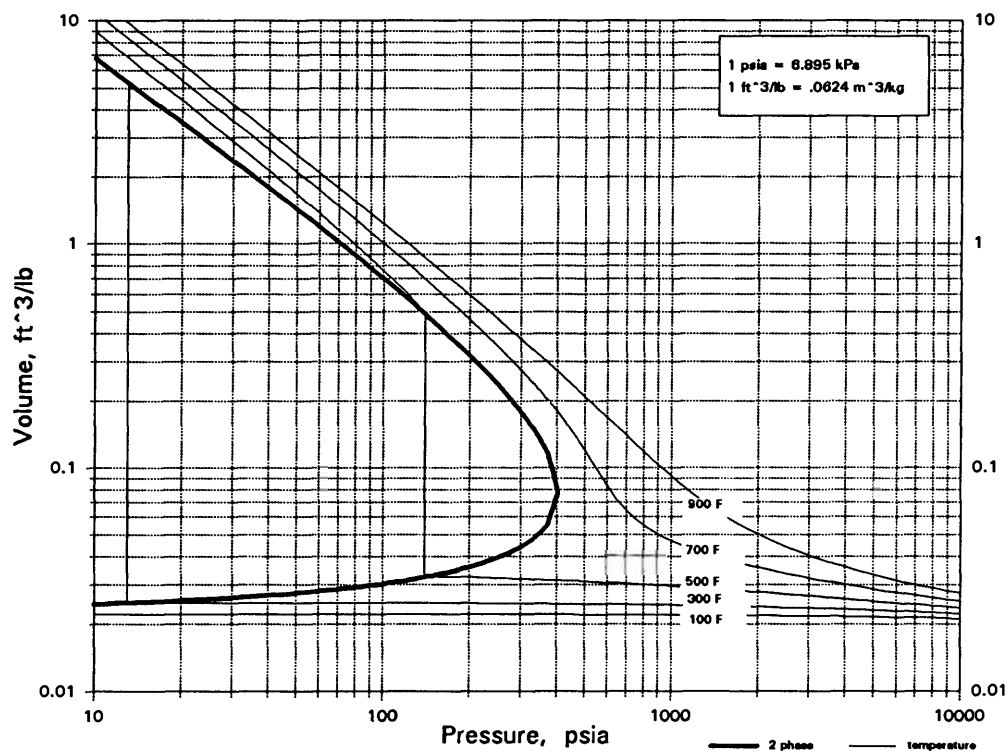


C7H14O

2-HEPTANONE

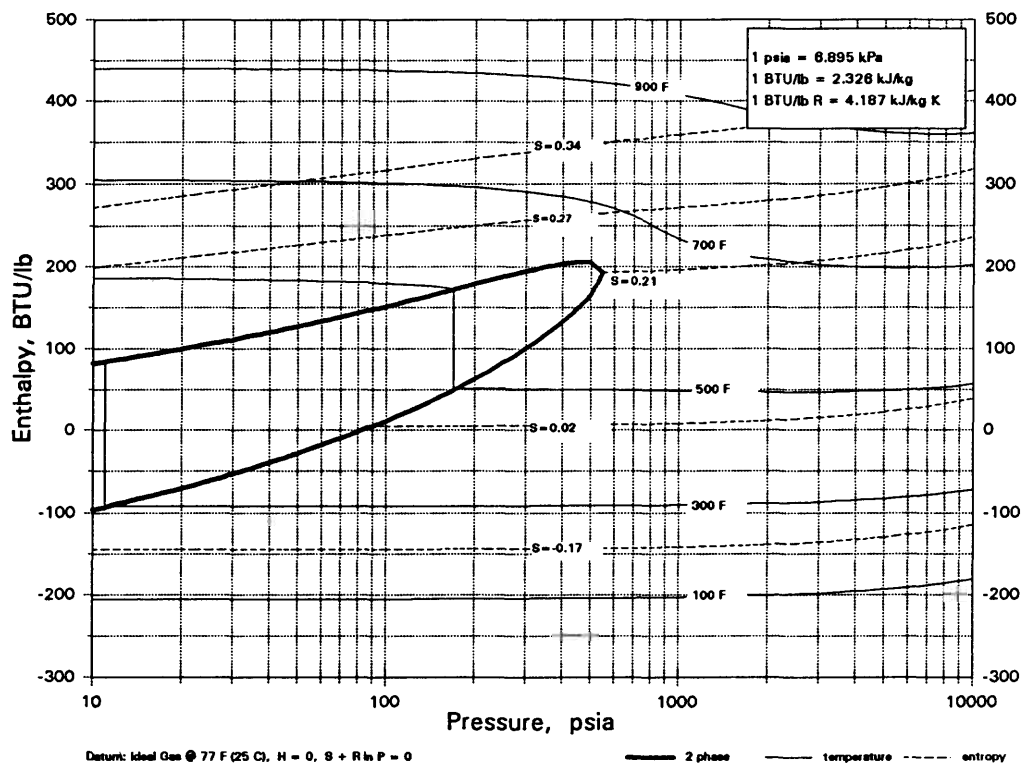
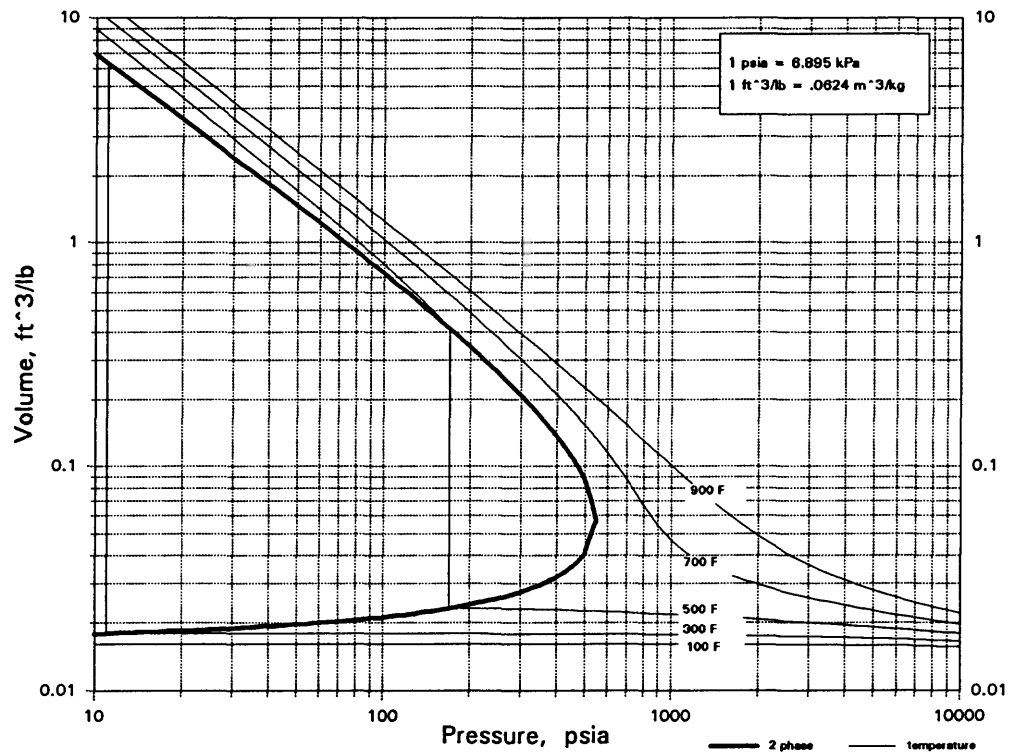


C7H14O
1-HEPTANAL

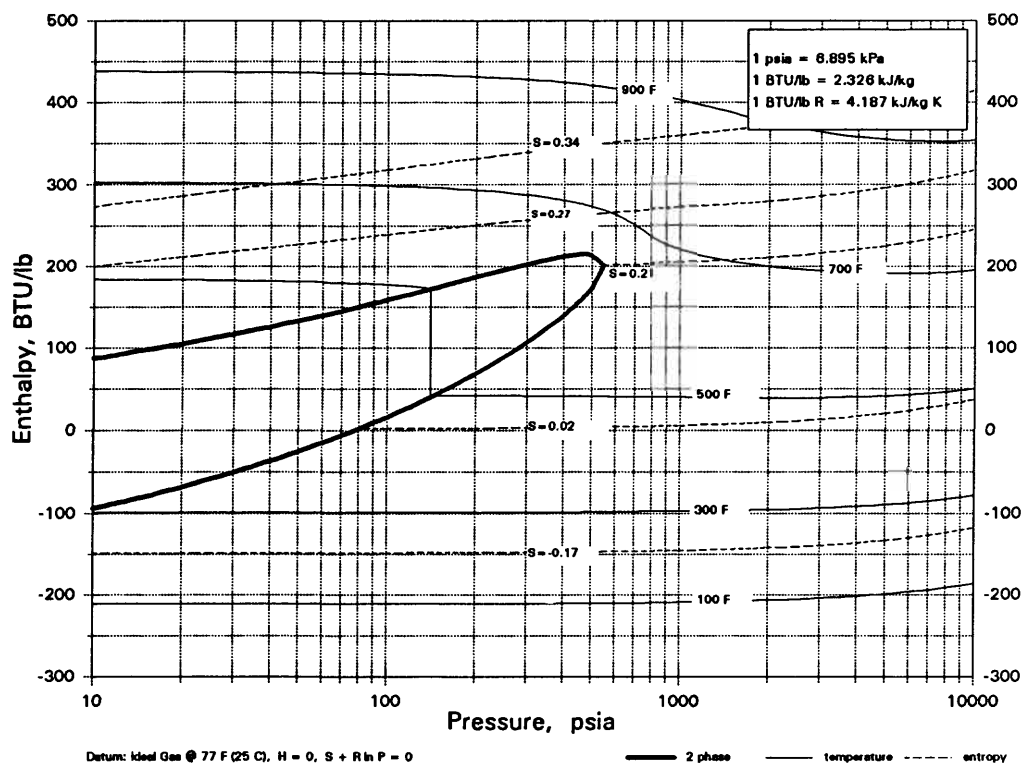
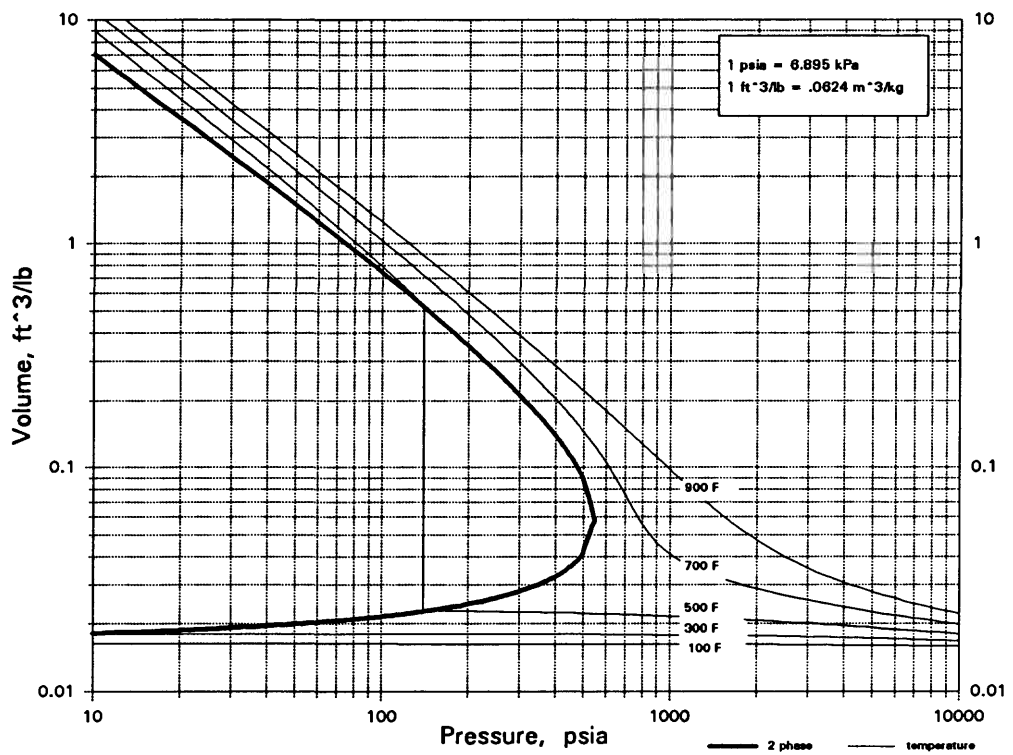


C7H14O

1-METHYLCYCLOHEXANOL

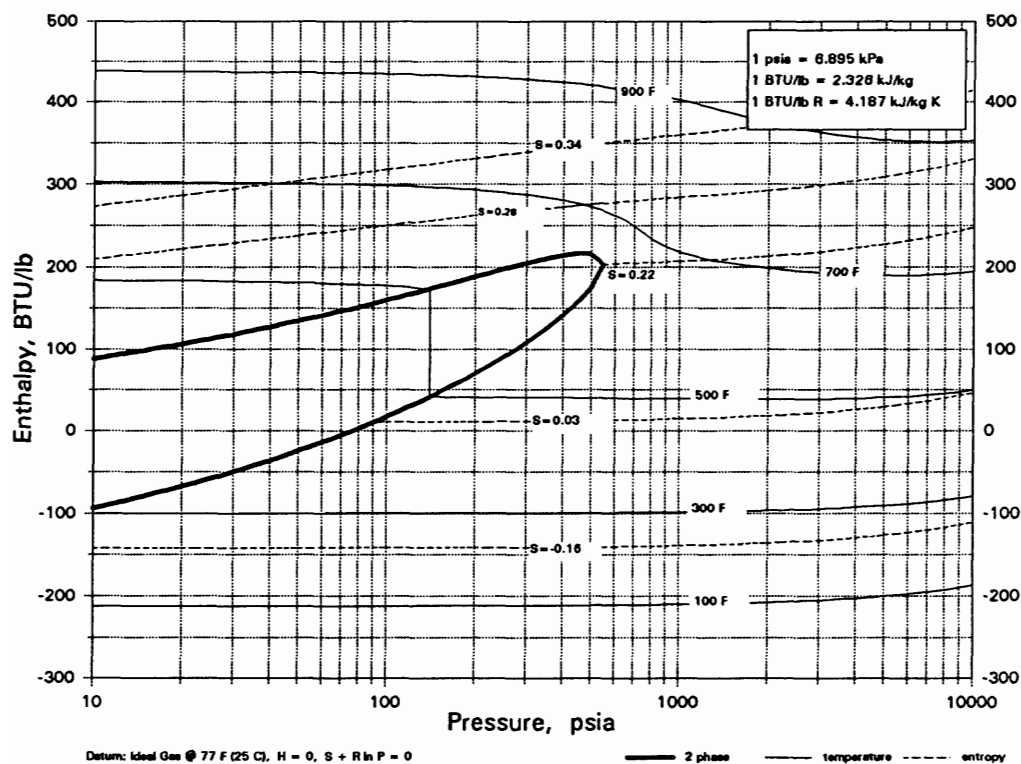
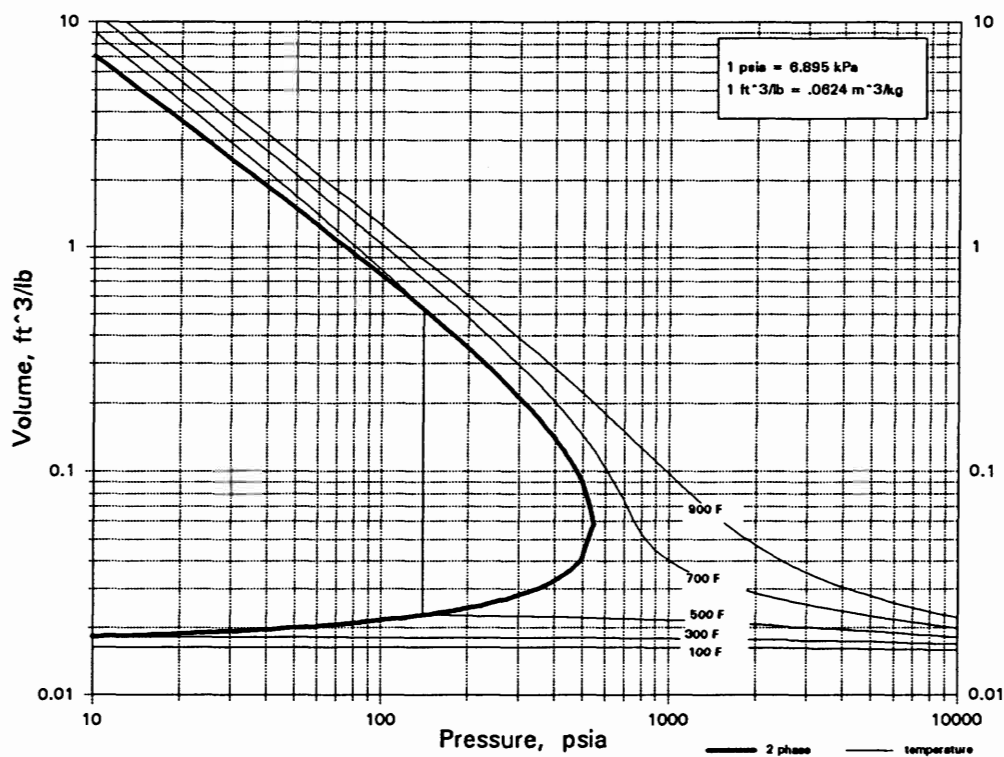


C7H14O
cis-2-METHYLCYCLOHEXANOL



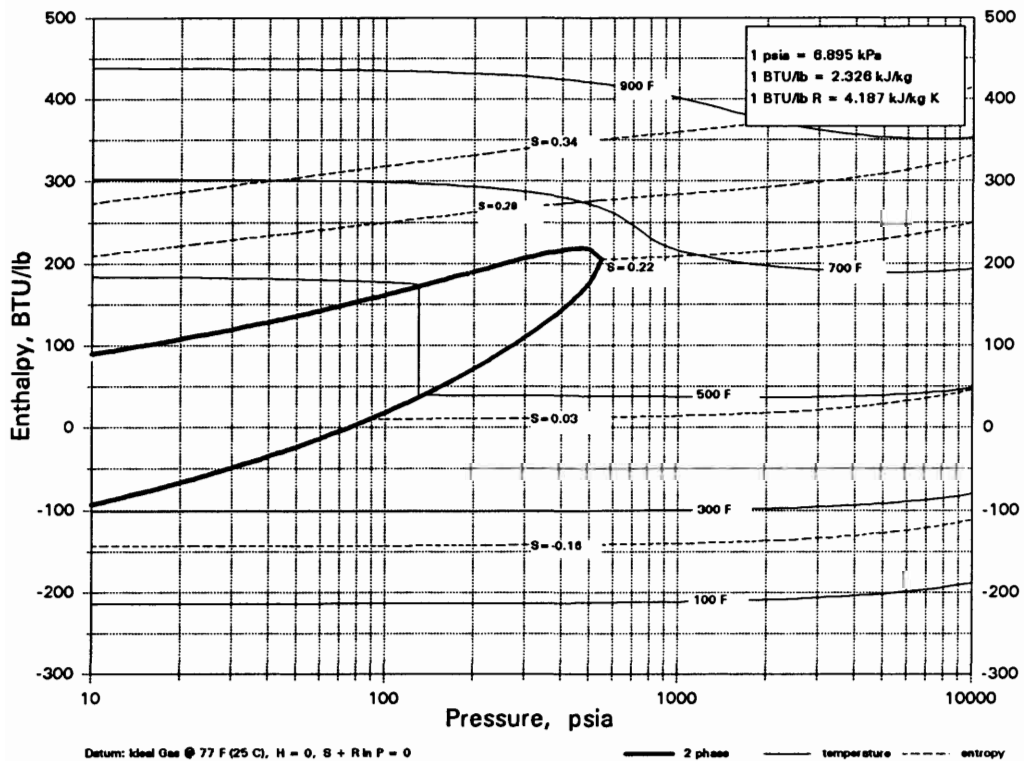
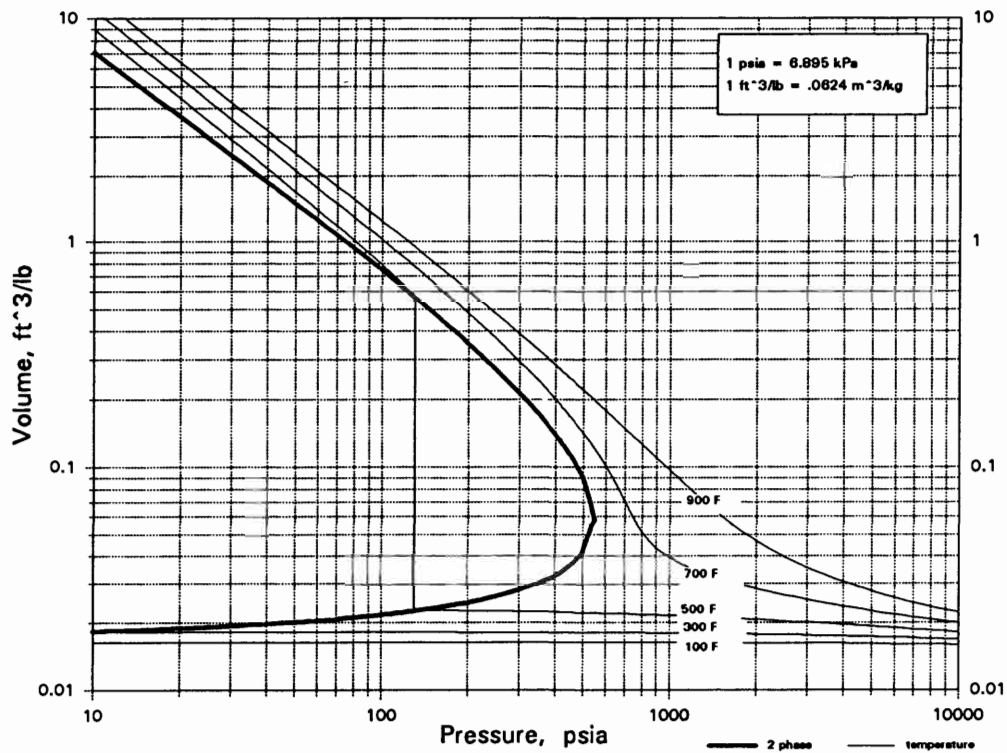
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trans-2-METHYLCYCLOHEXANOL



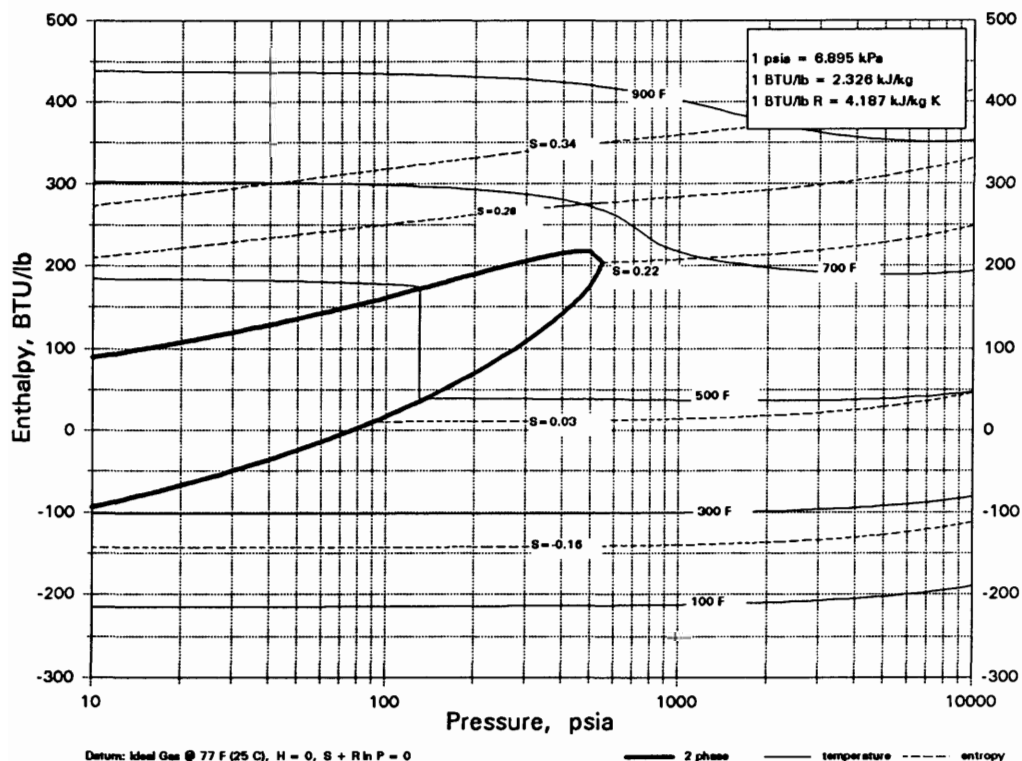
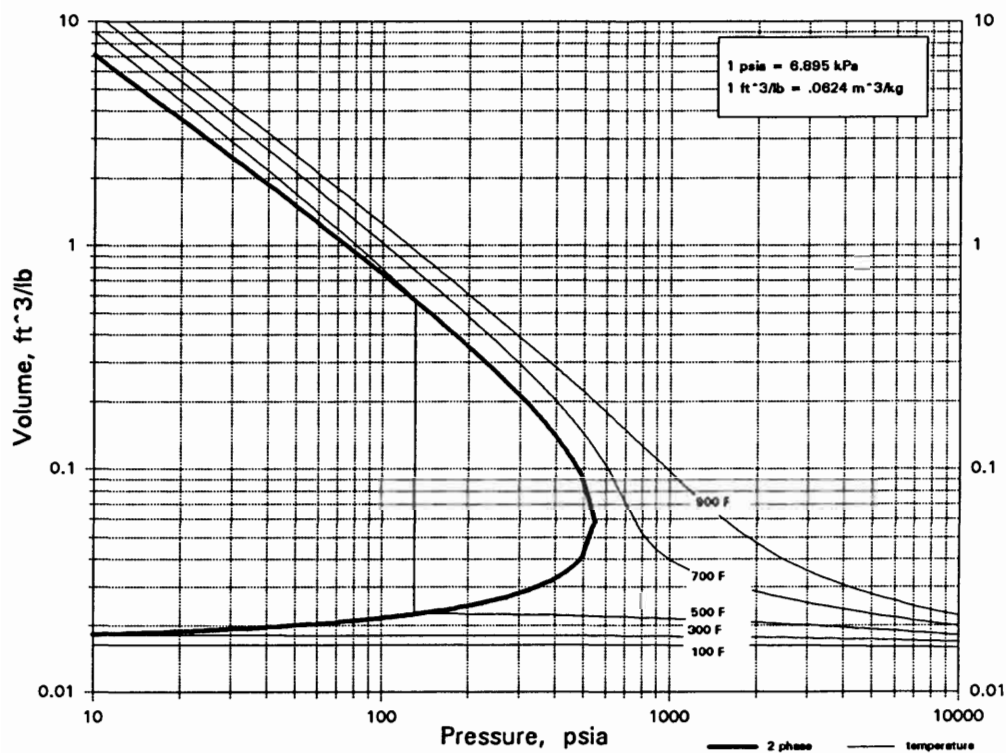
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cis-3-METHYLCYCLOHEXANOL



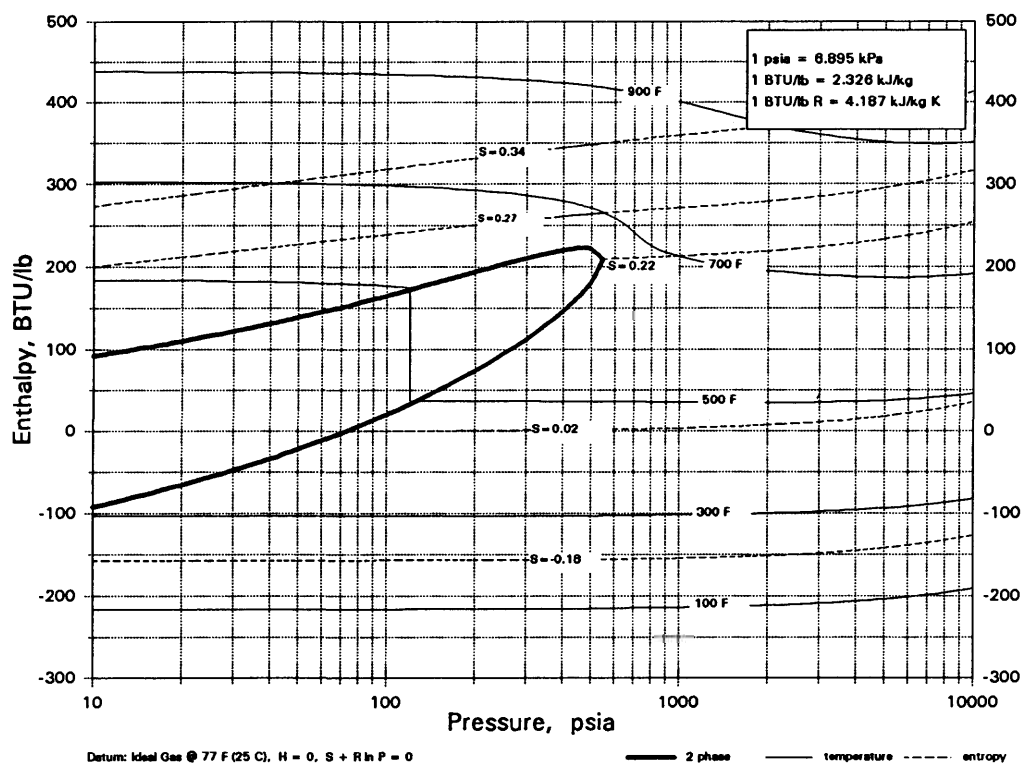
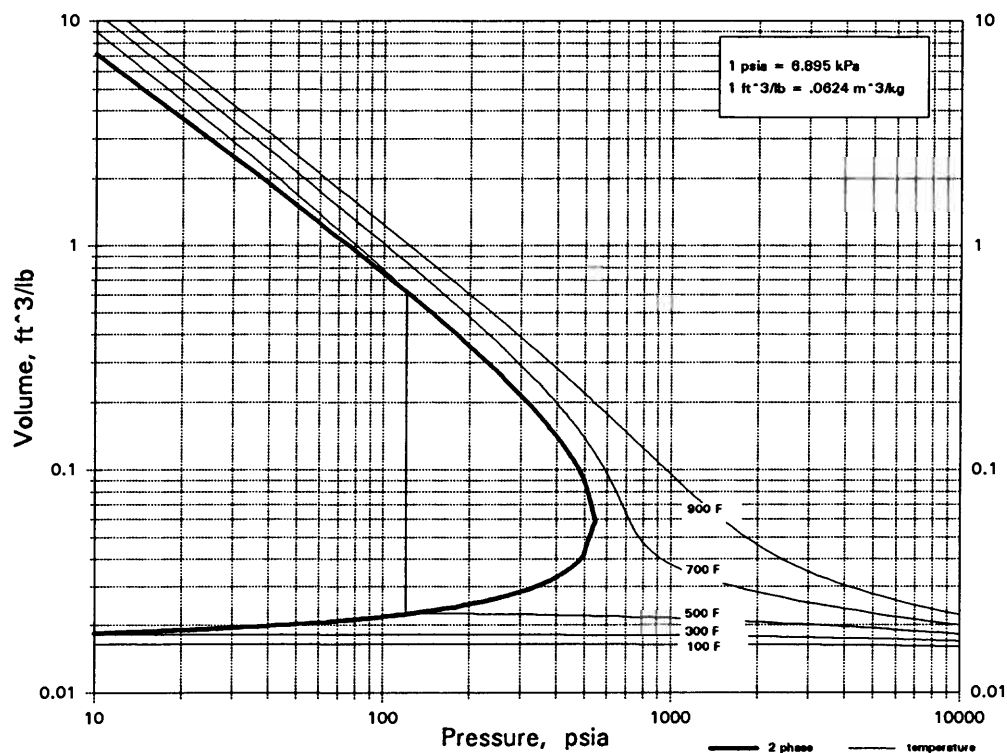
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trans-3-METHYLCYCLOHEXANOL



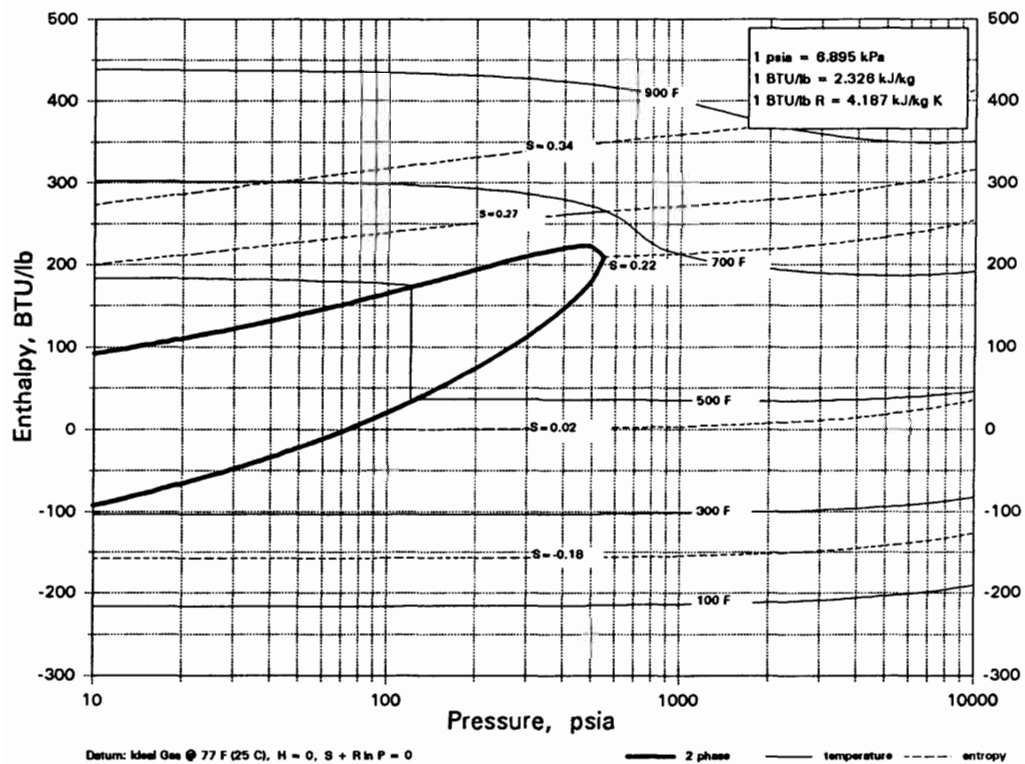
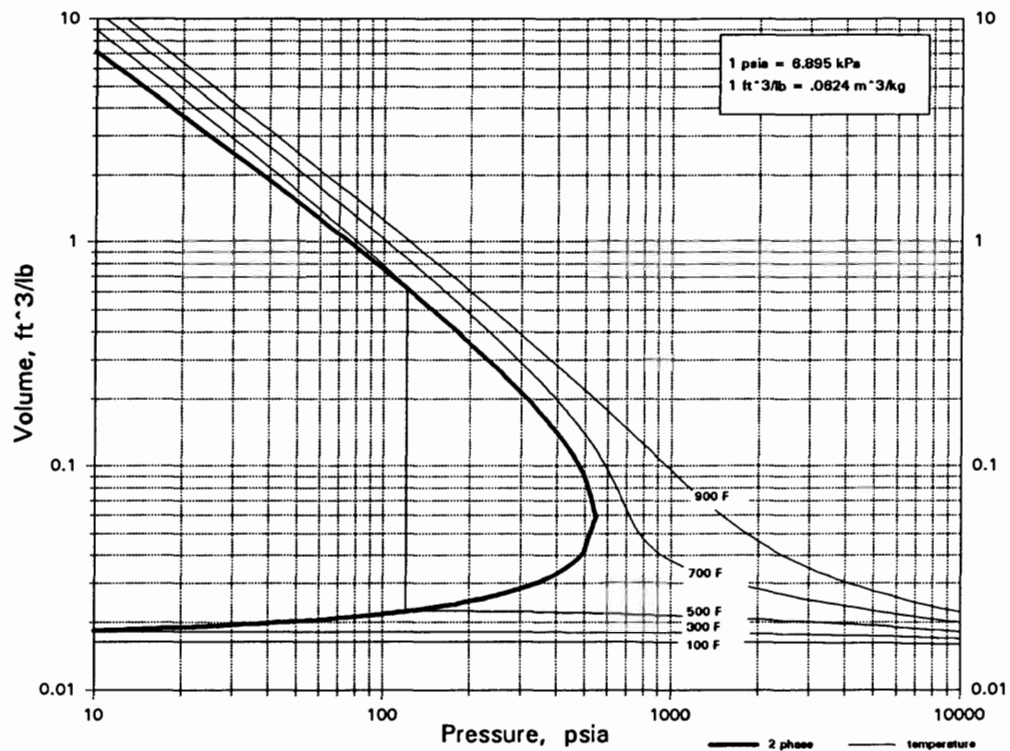
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cis-4-METHYLCYCLOHEXANOL



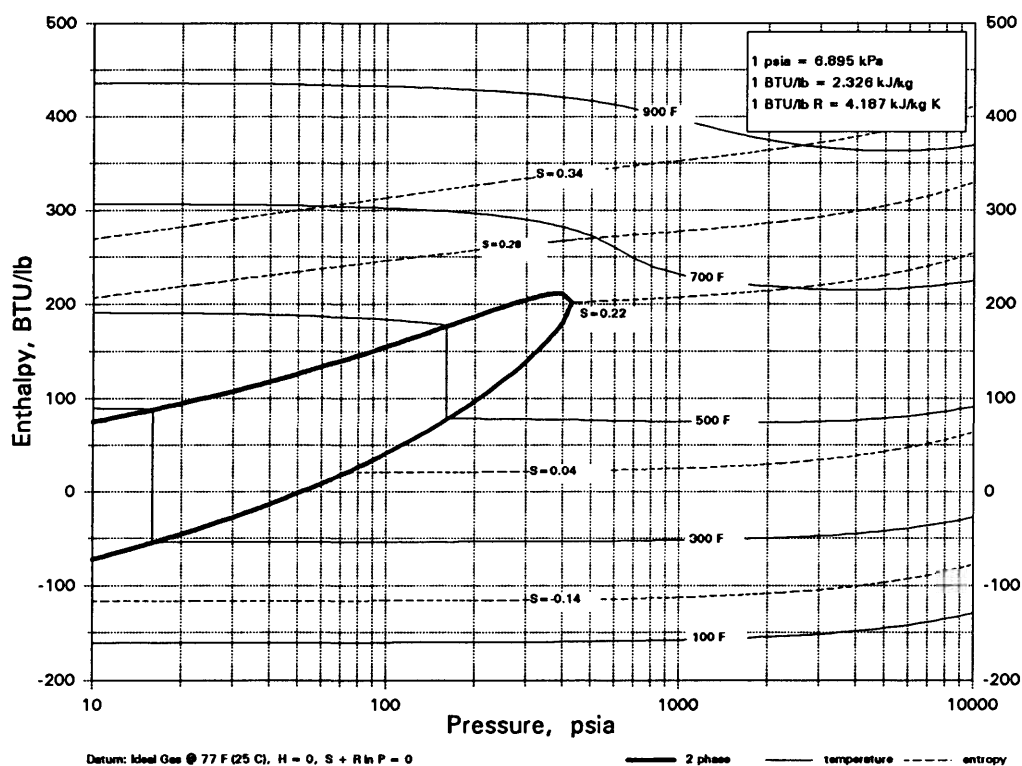
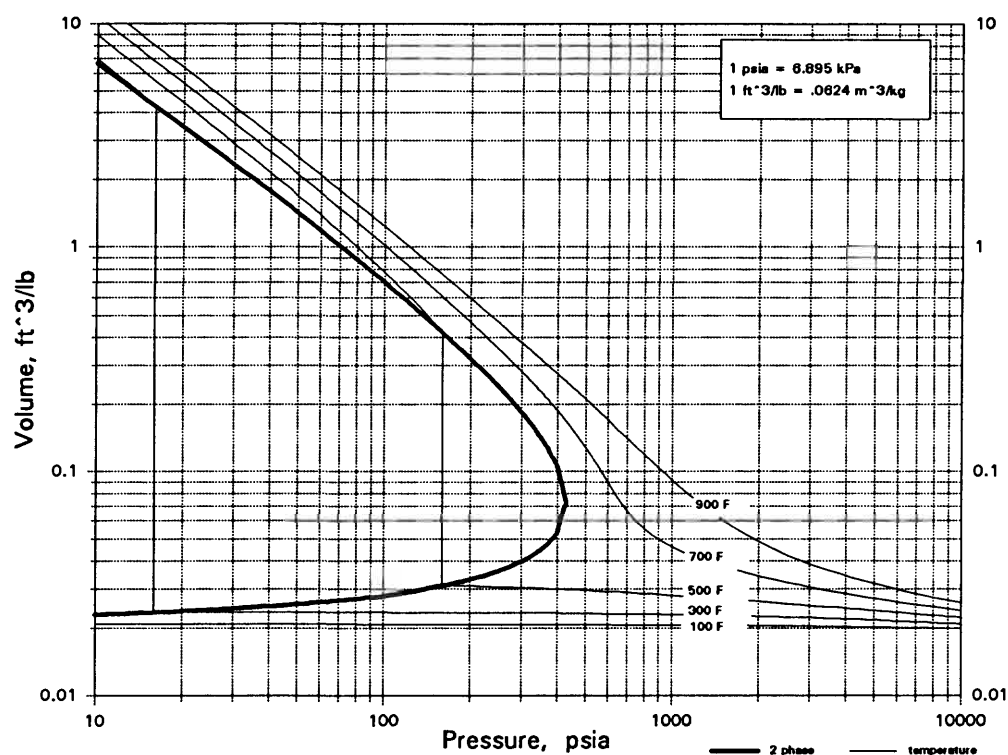
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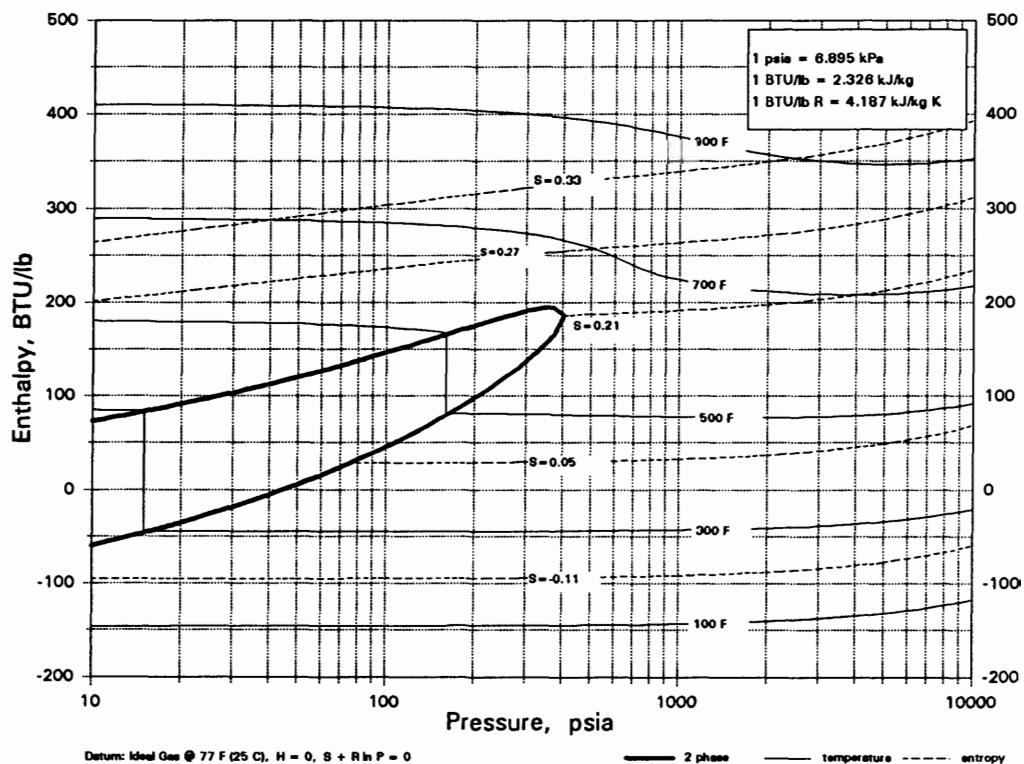
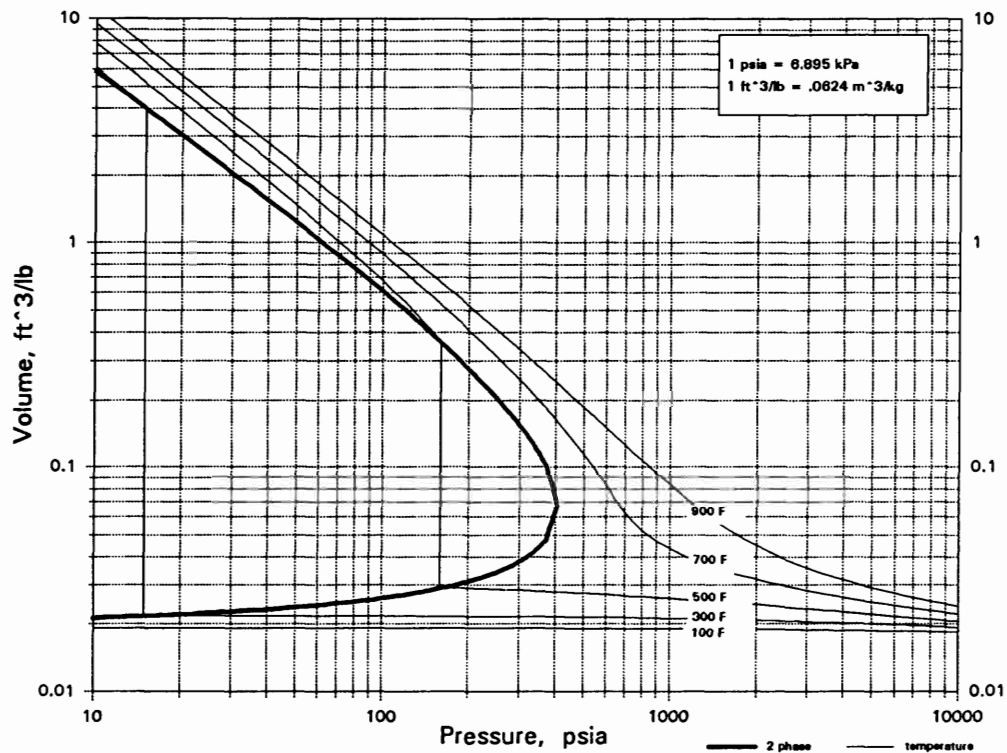
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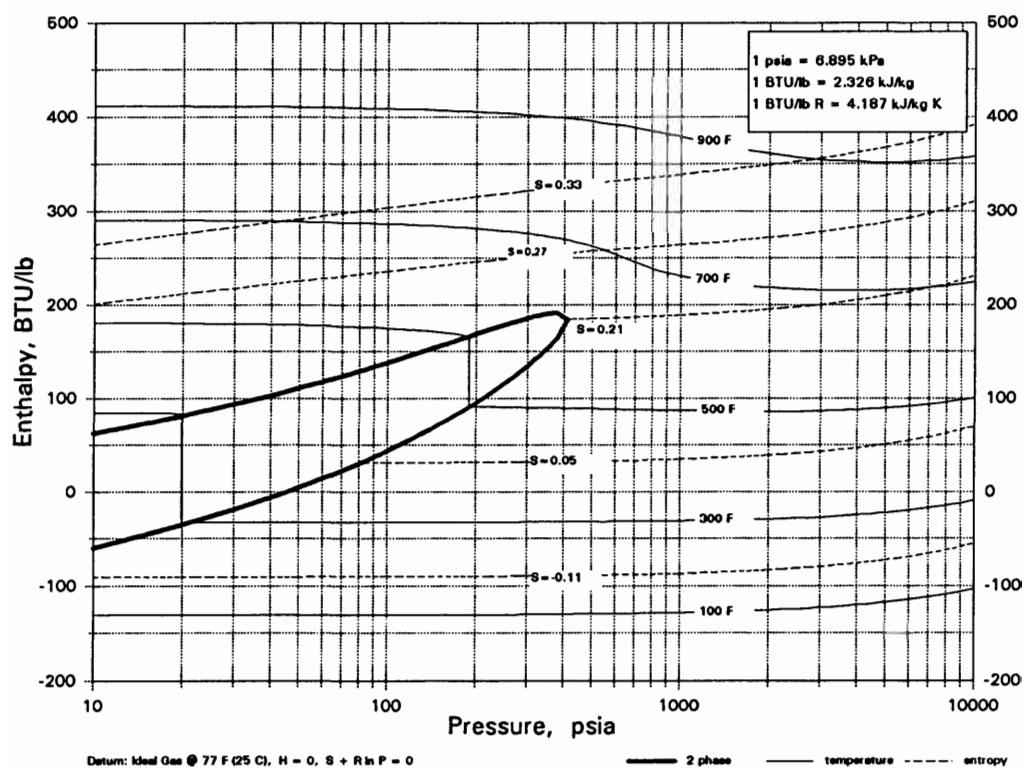
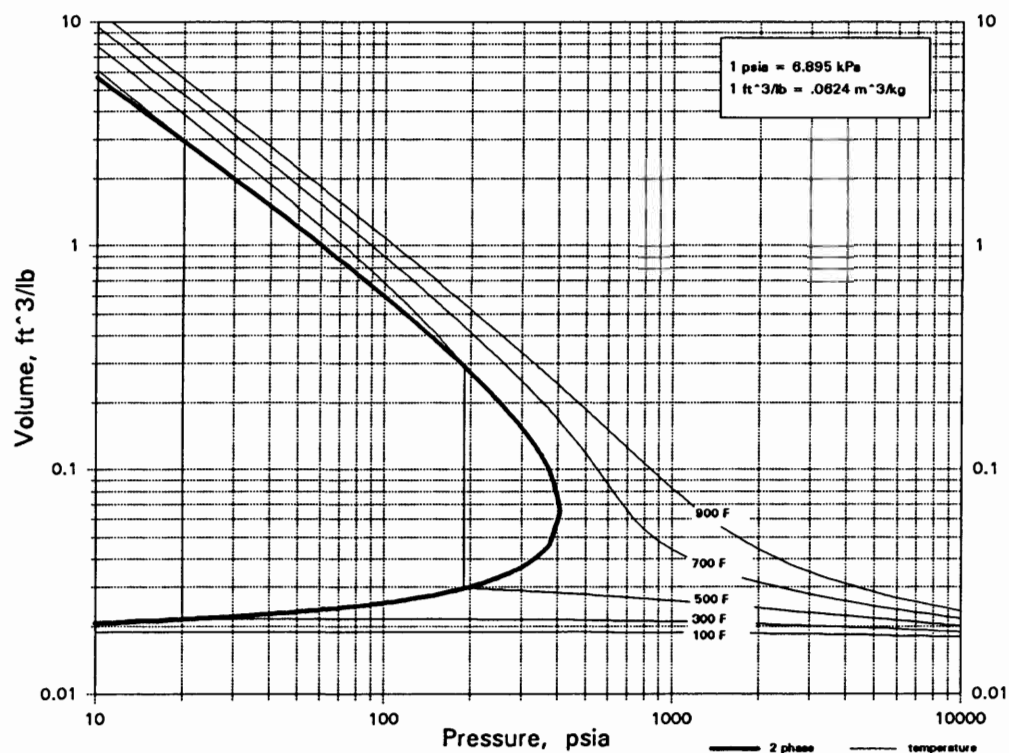
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n-BUTYL PROPIONATE



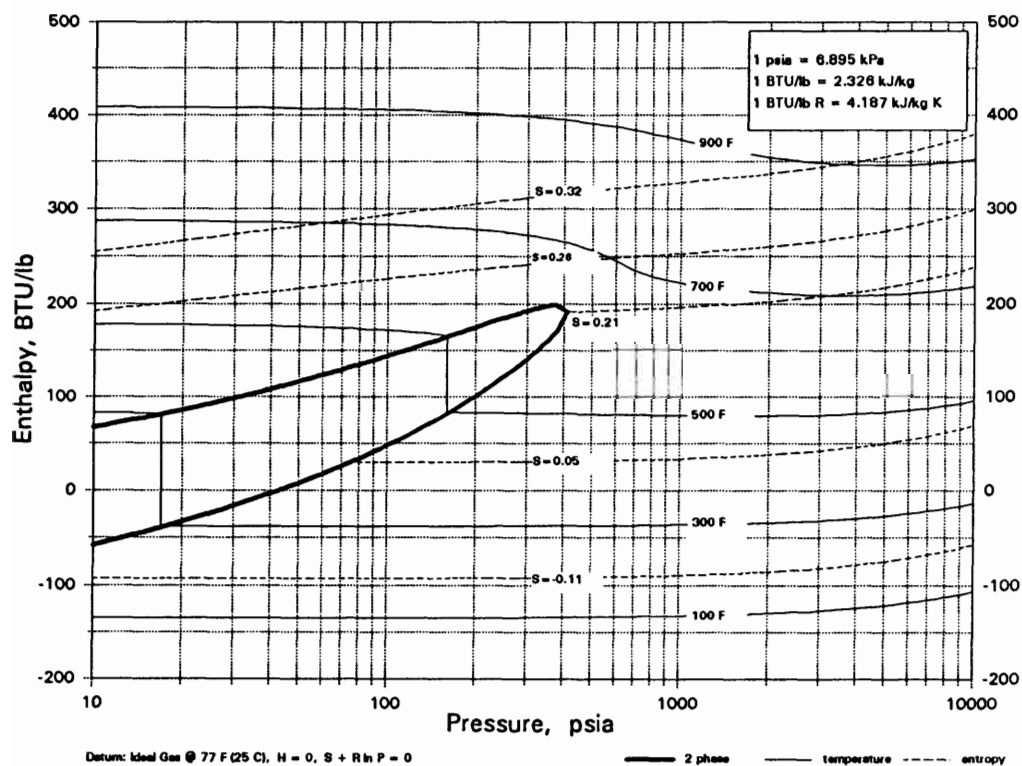
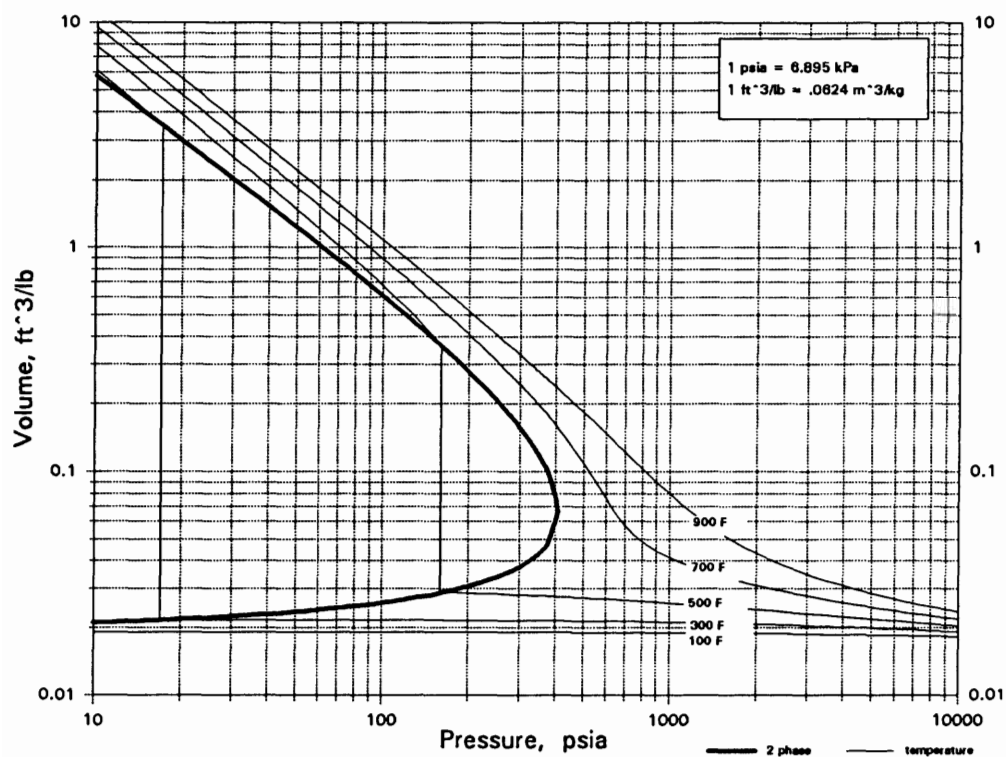
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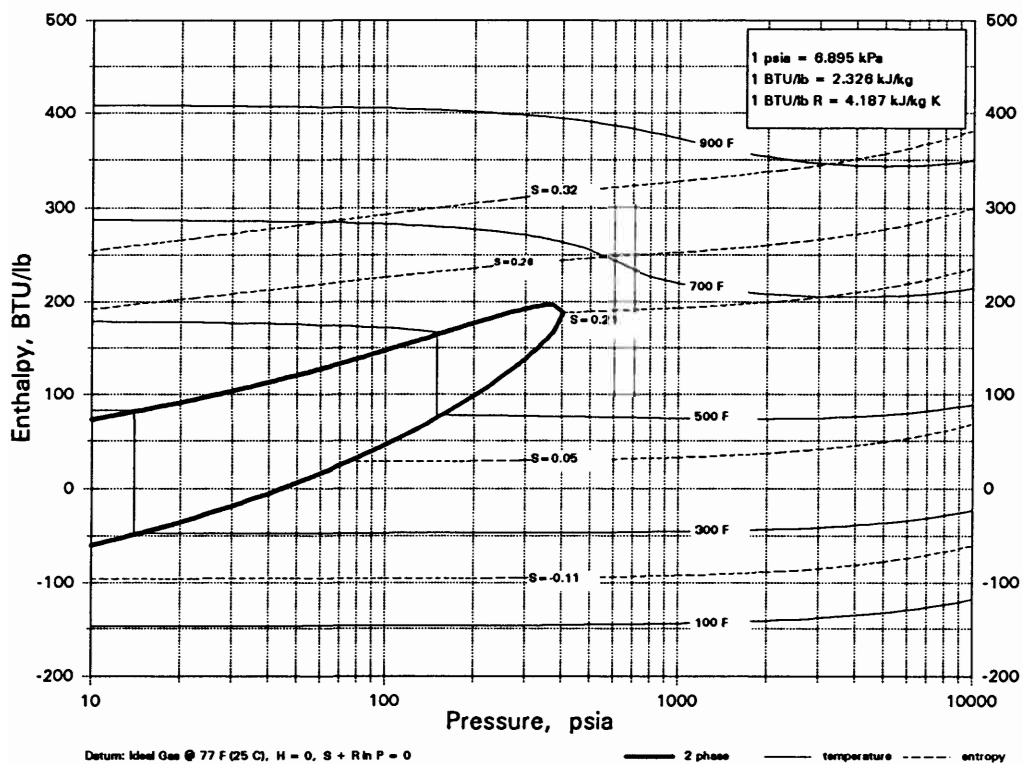
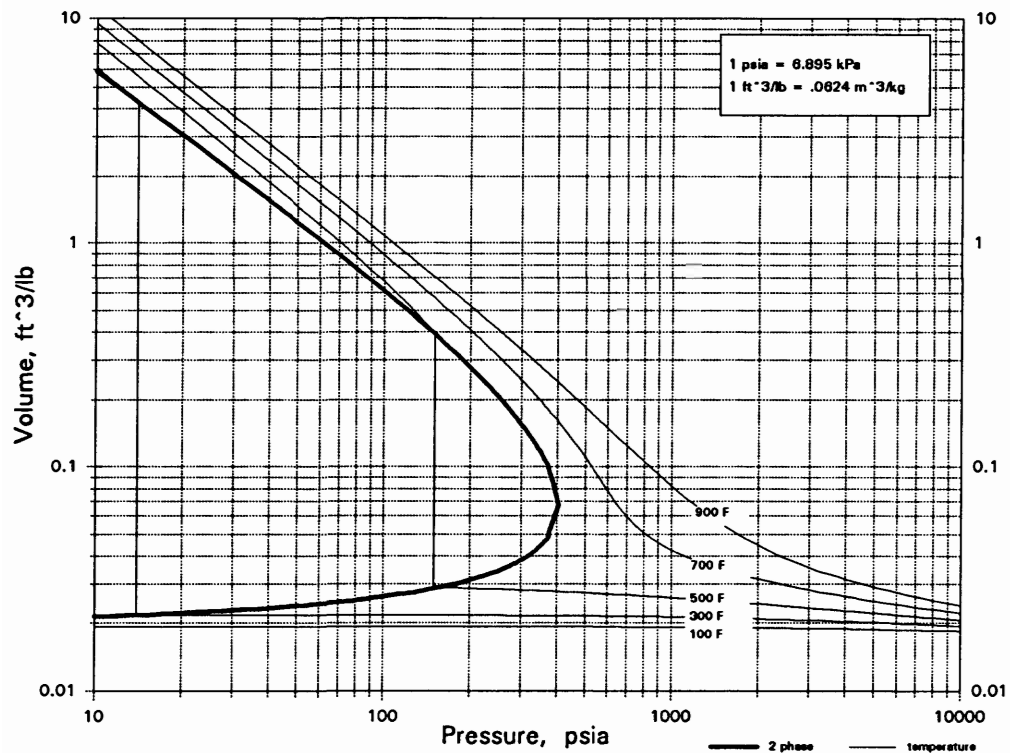
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ISOPENTYL ACETATE



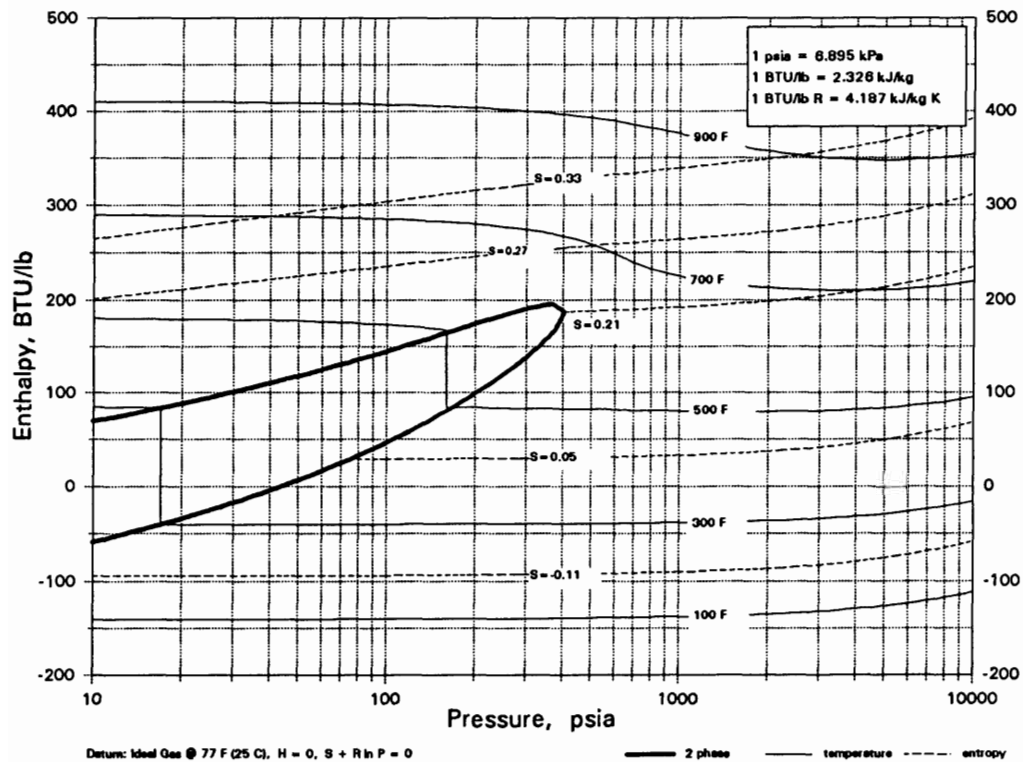
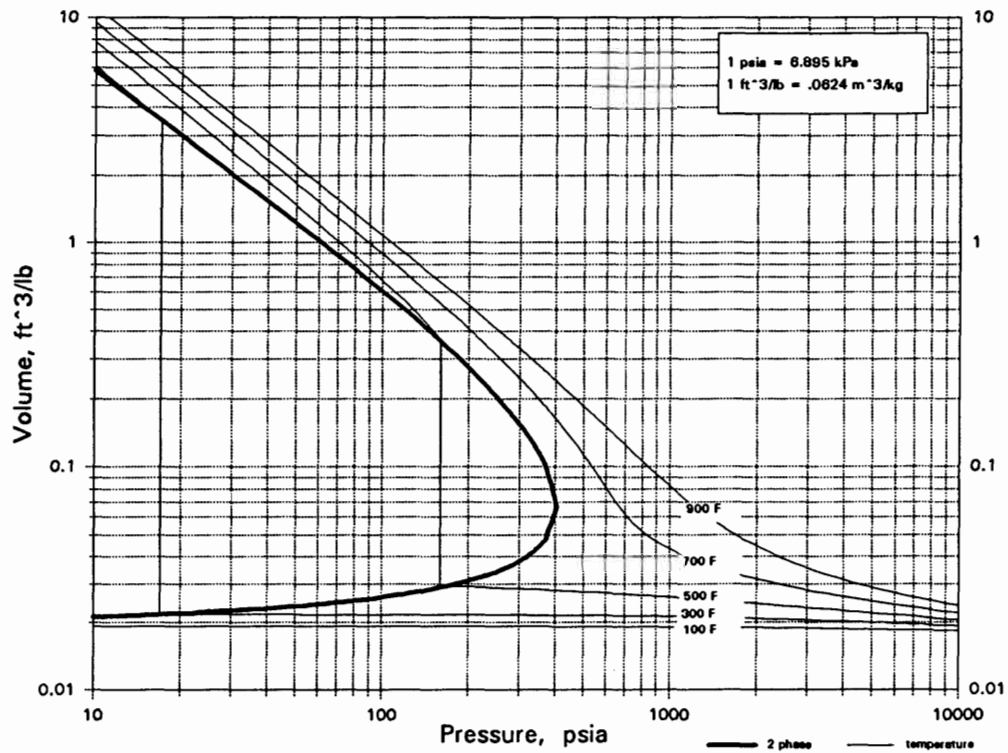
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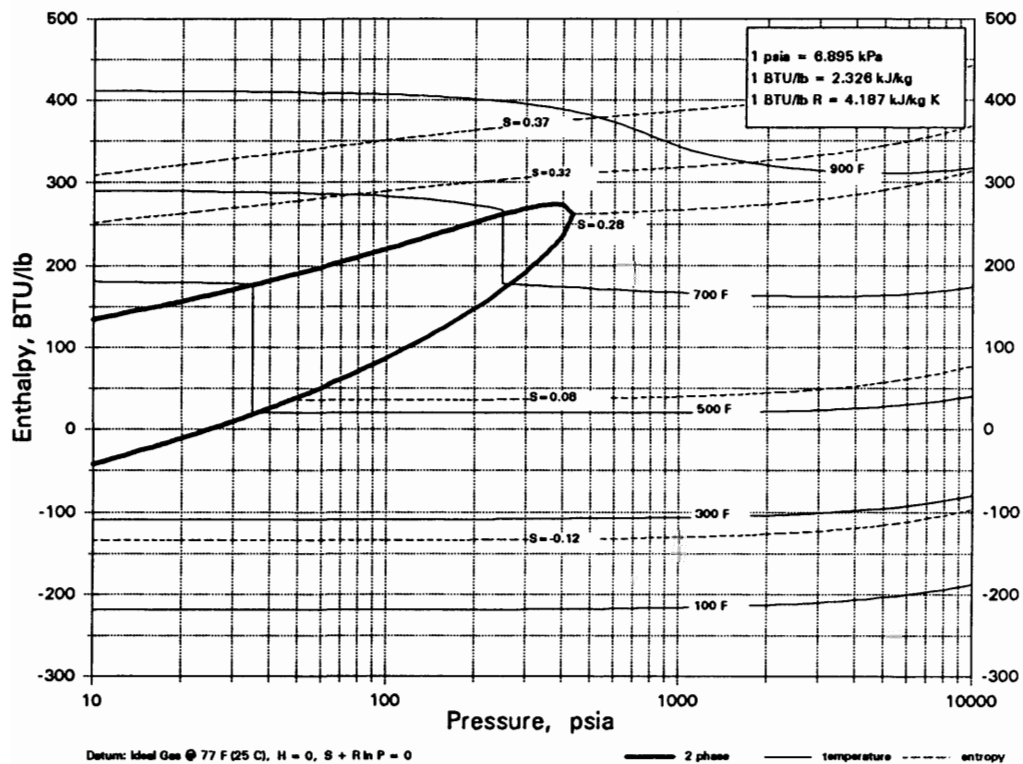
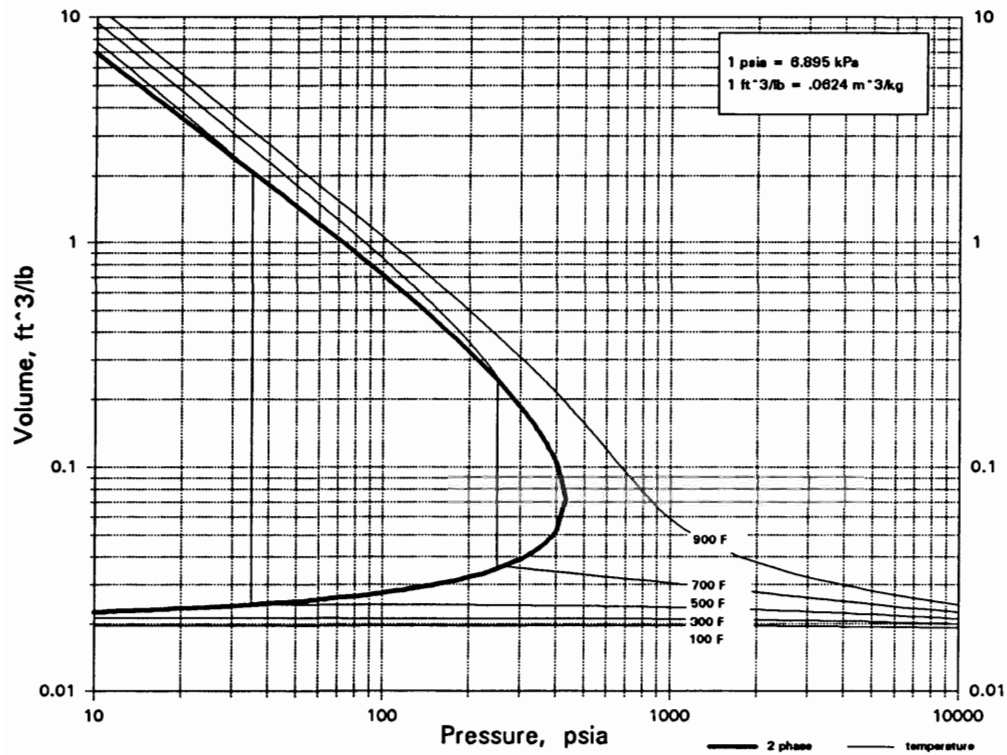
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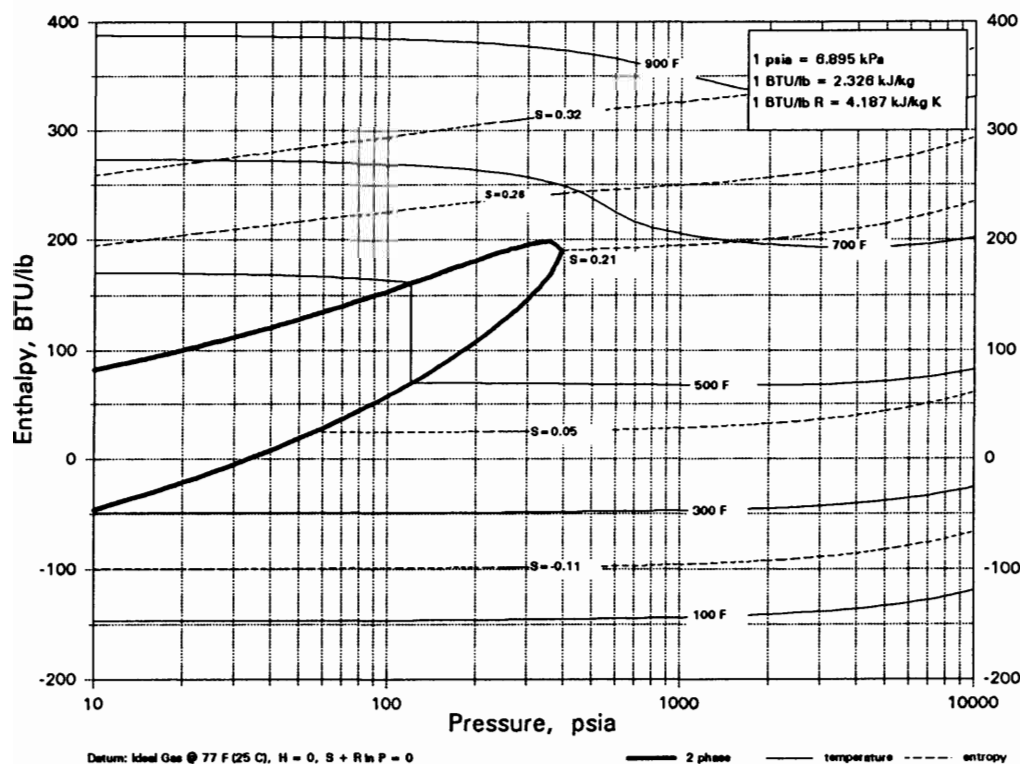


C7H14O2

n-HEPTANOIC ACID

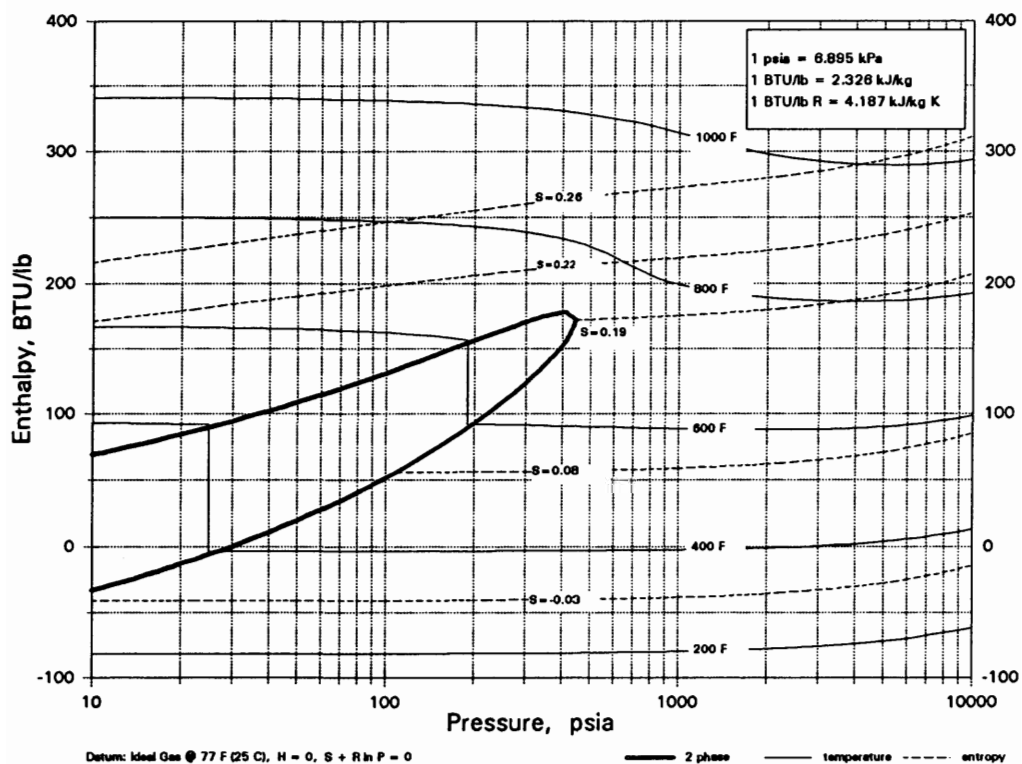
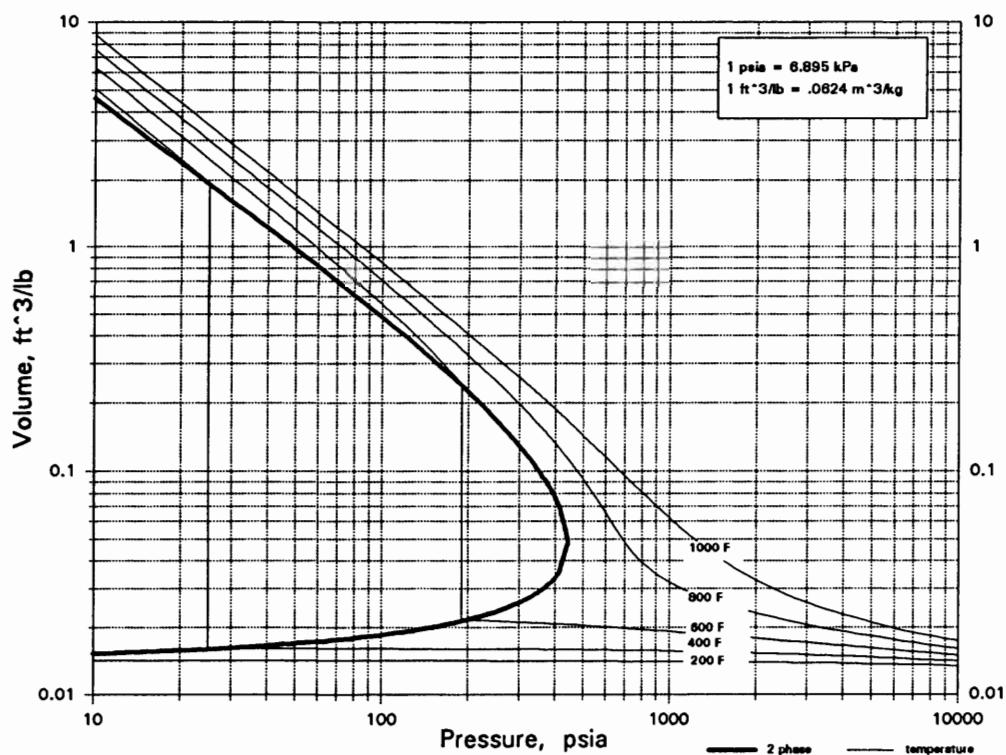


ETHYL-3-ETHOXYPROPIONATE

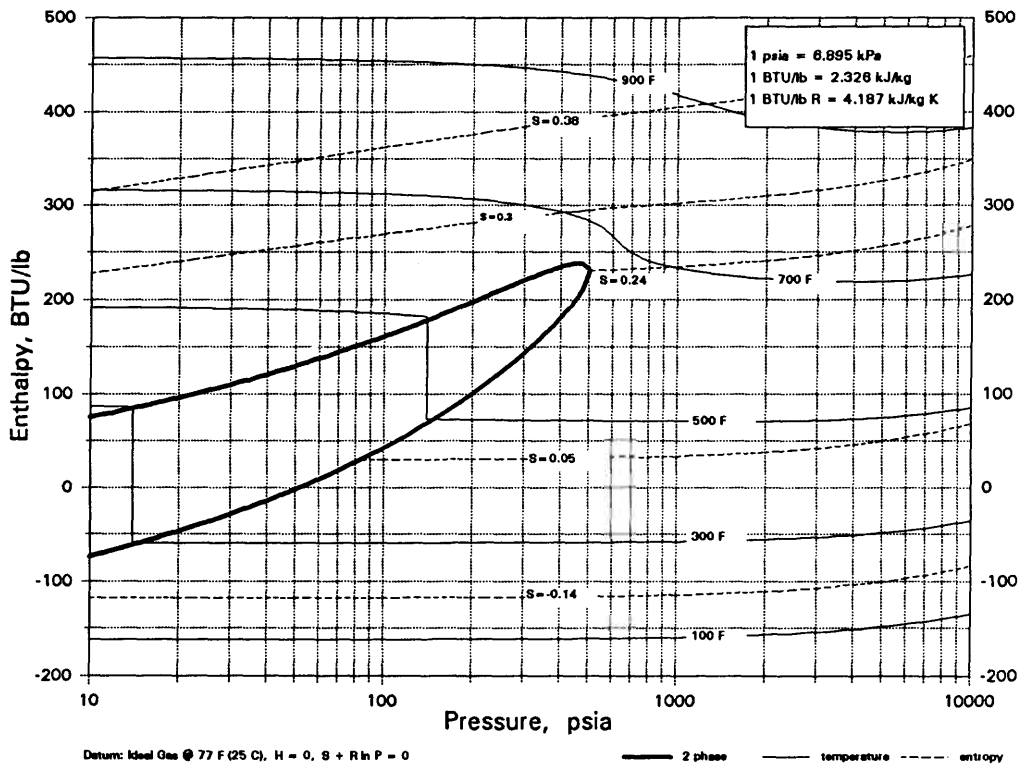
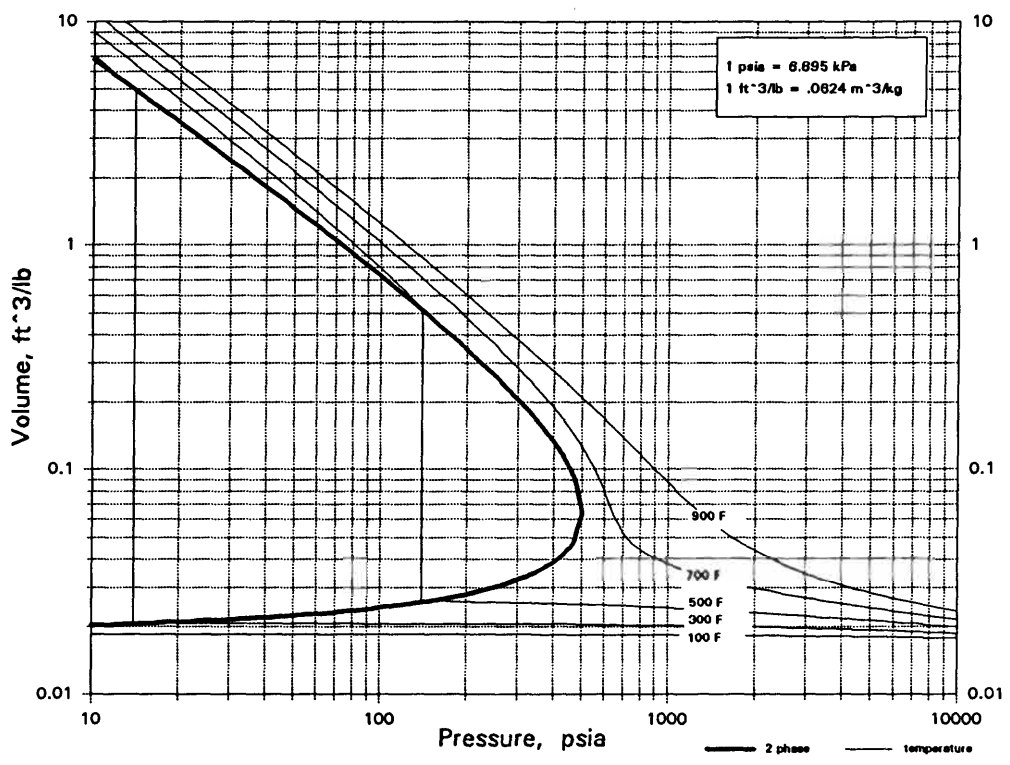


C7H15Br

1-BROMOHEPTANE

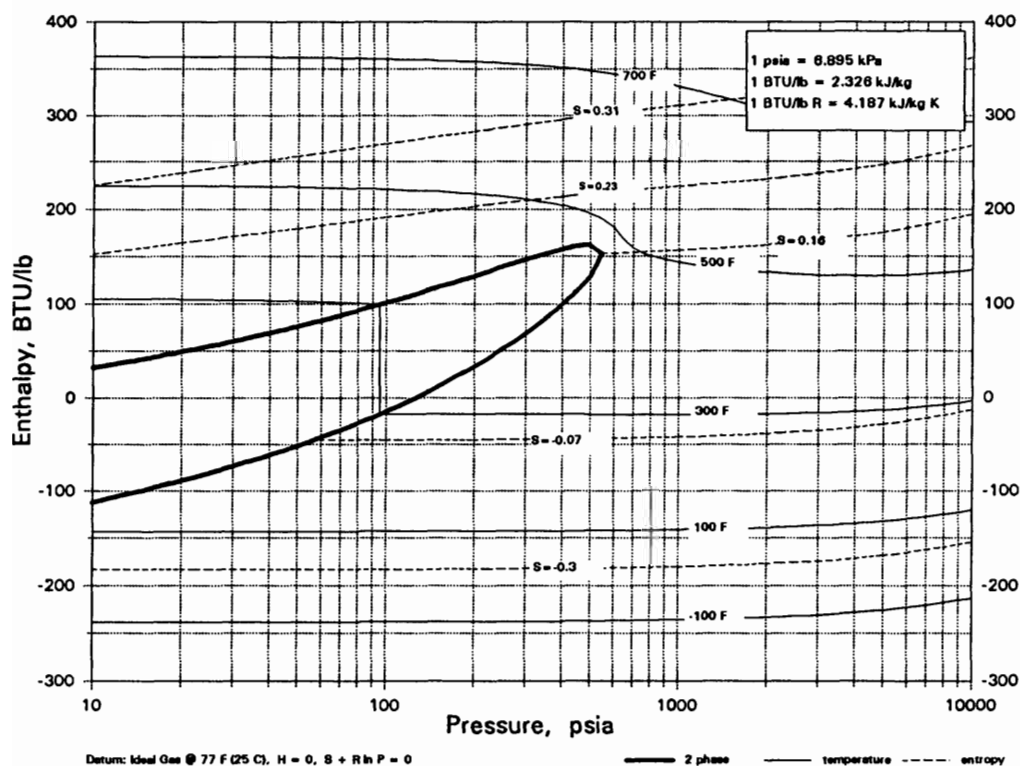
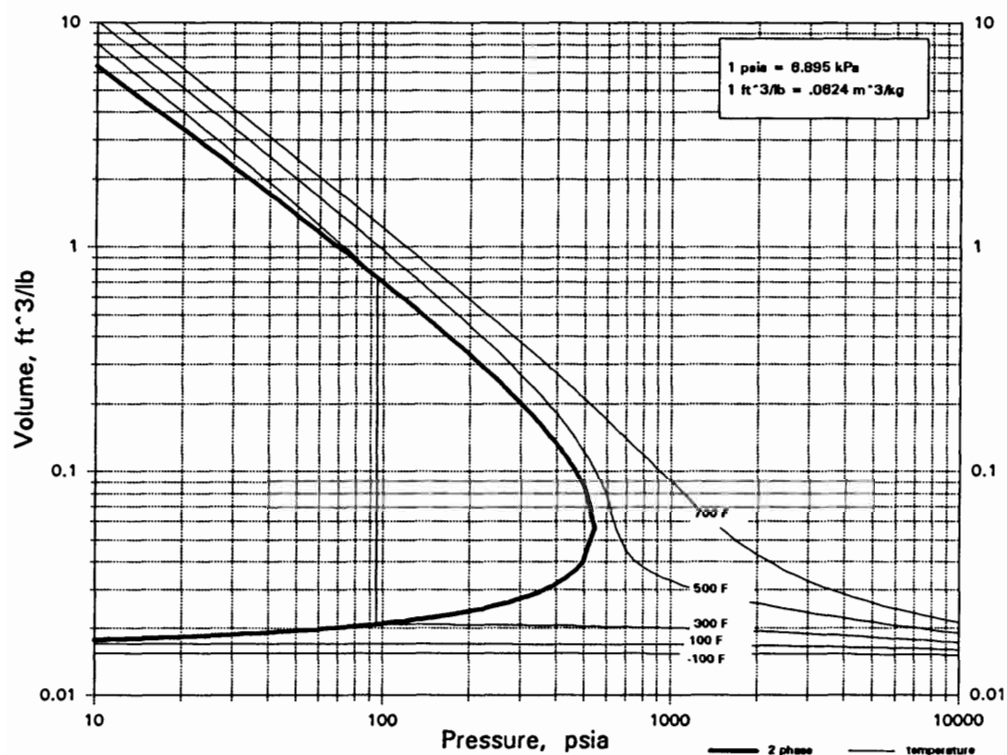


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N-METHYLCYCLOHEXYLAMINE



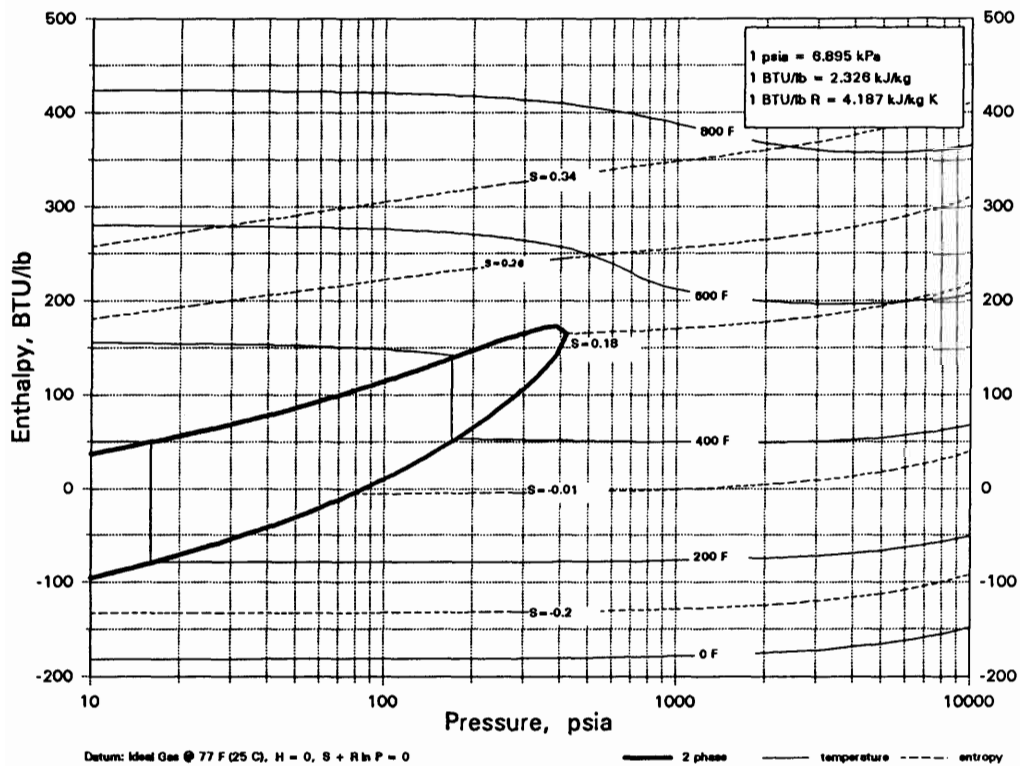
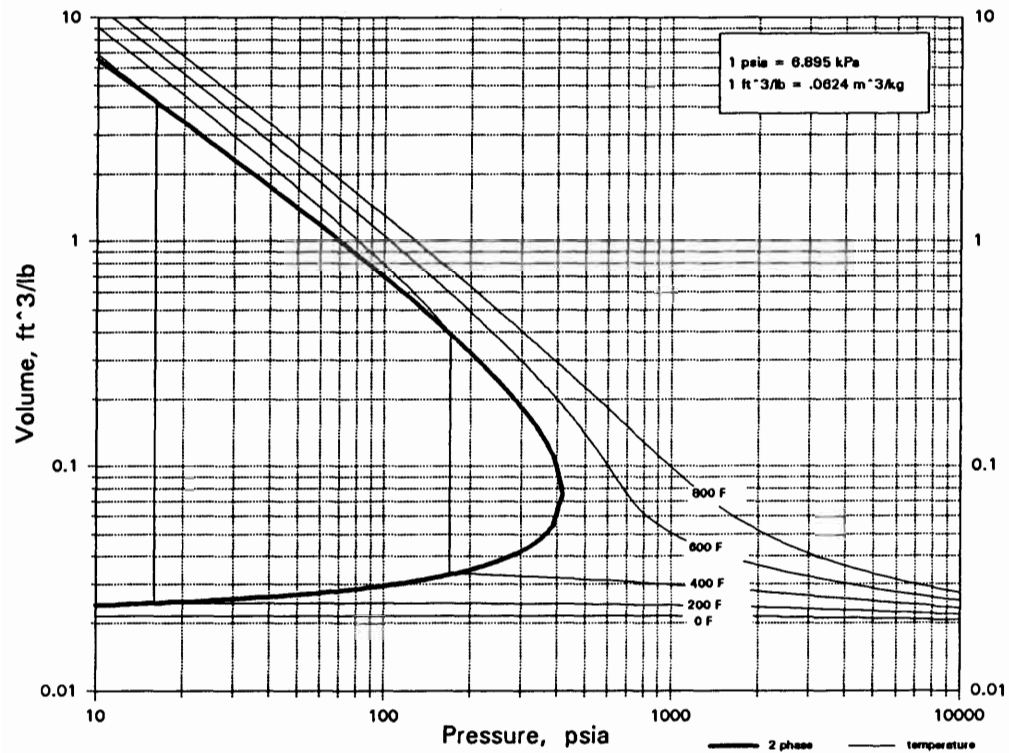
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2-2-DIMETHYLPENTANE

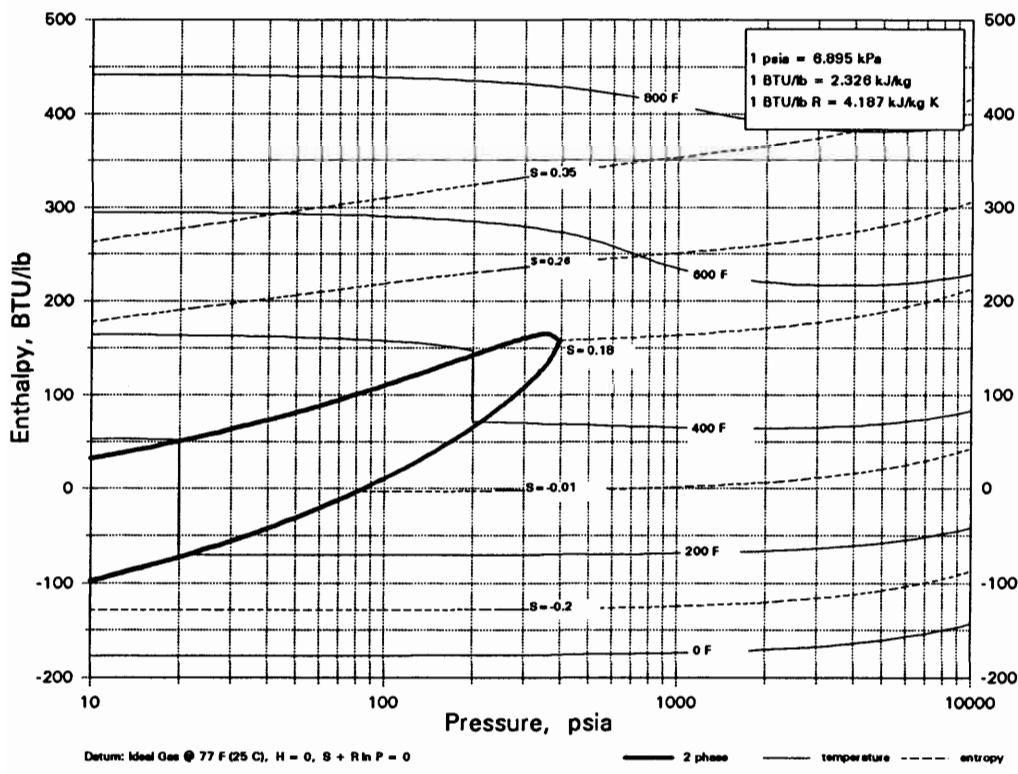
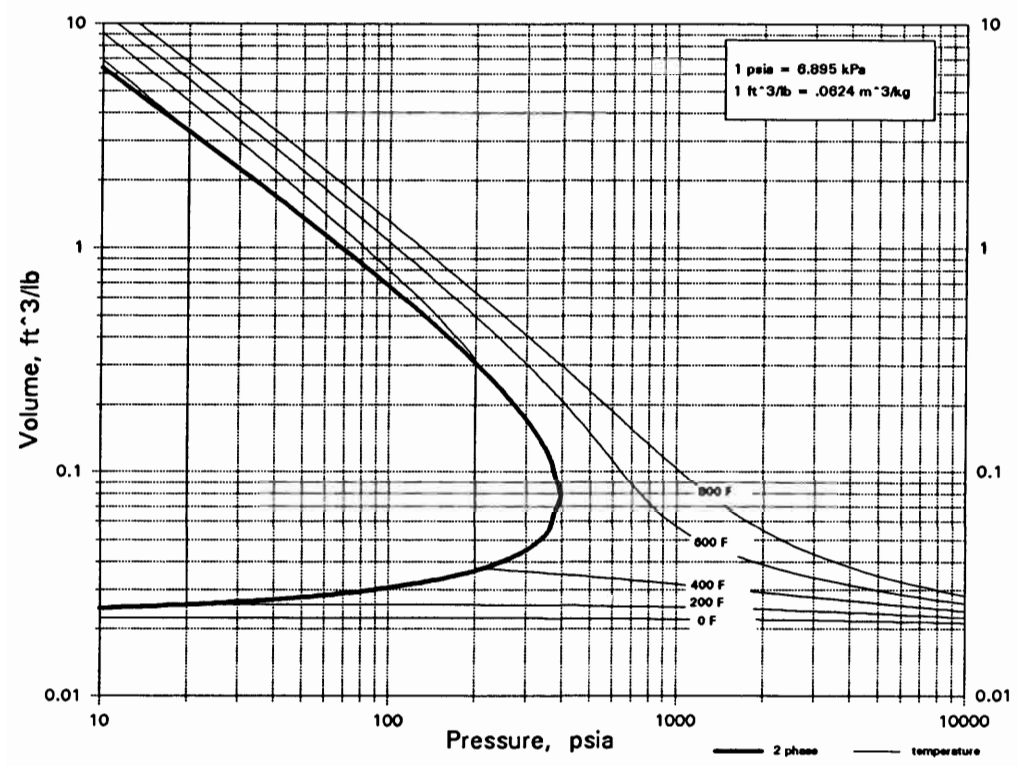


C7H16

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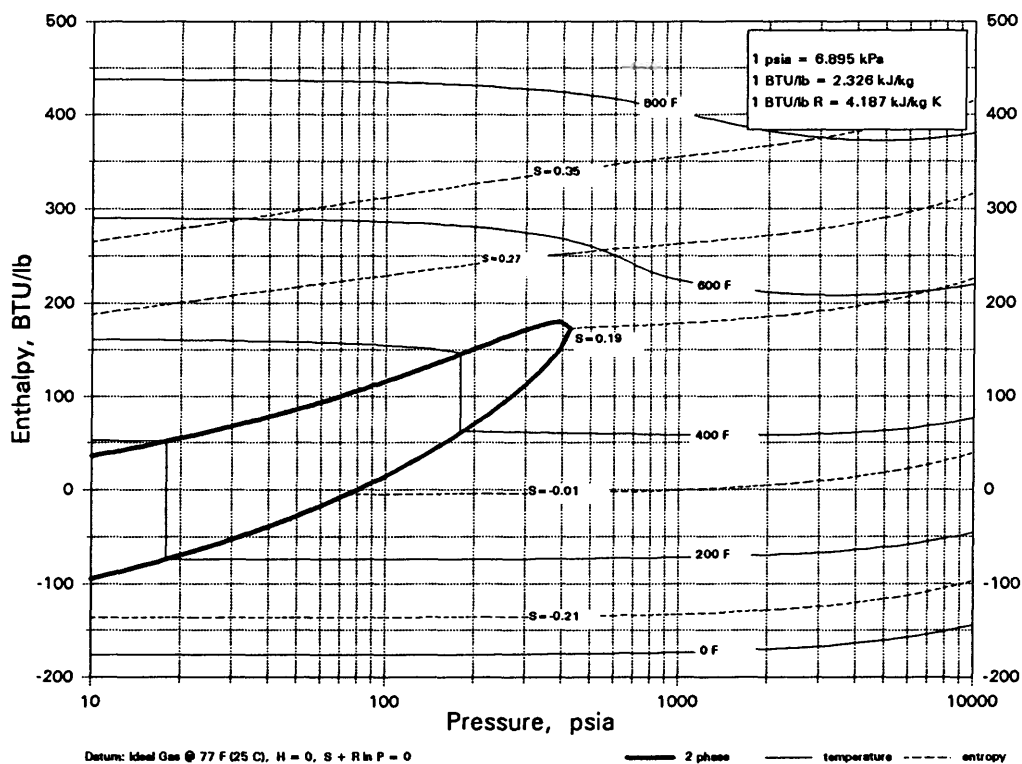
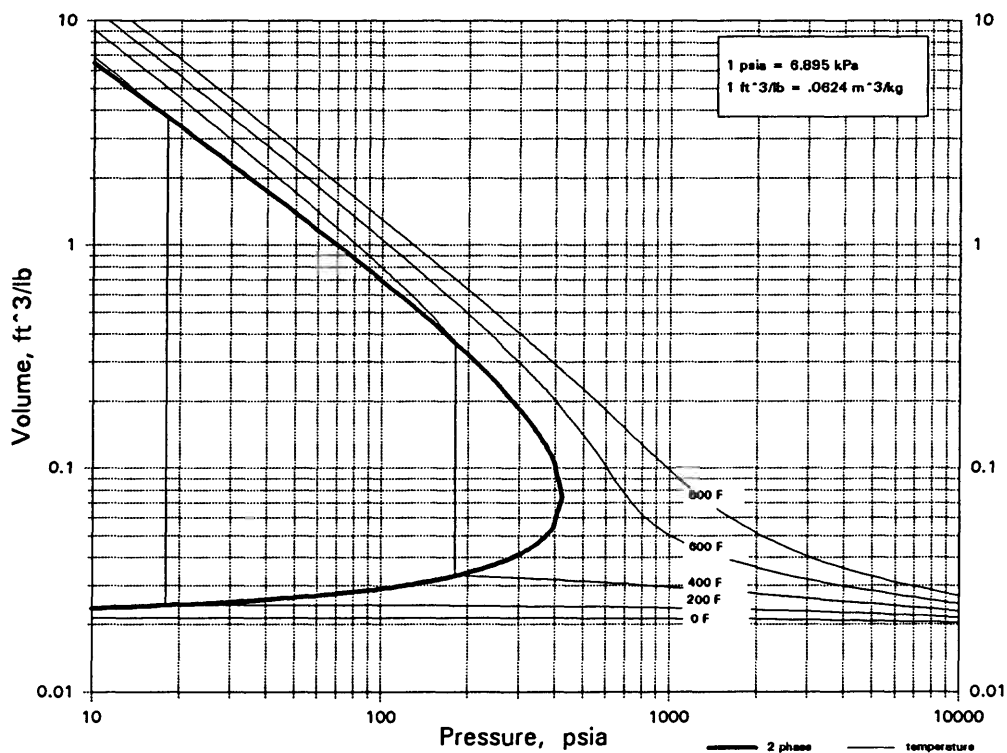


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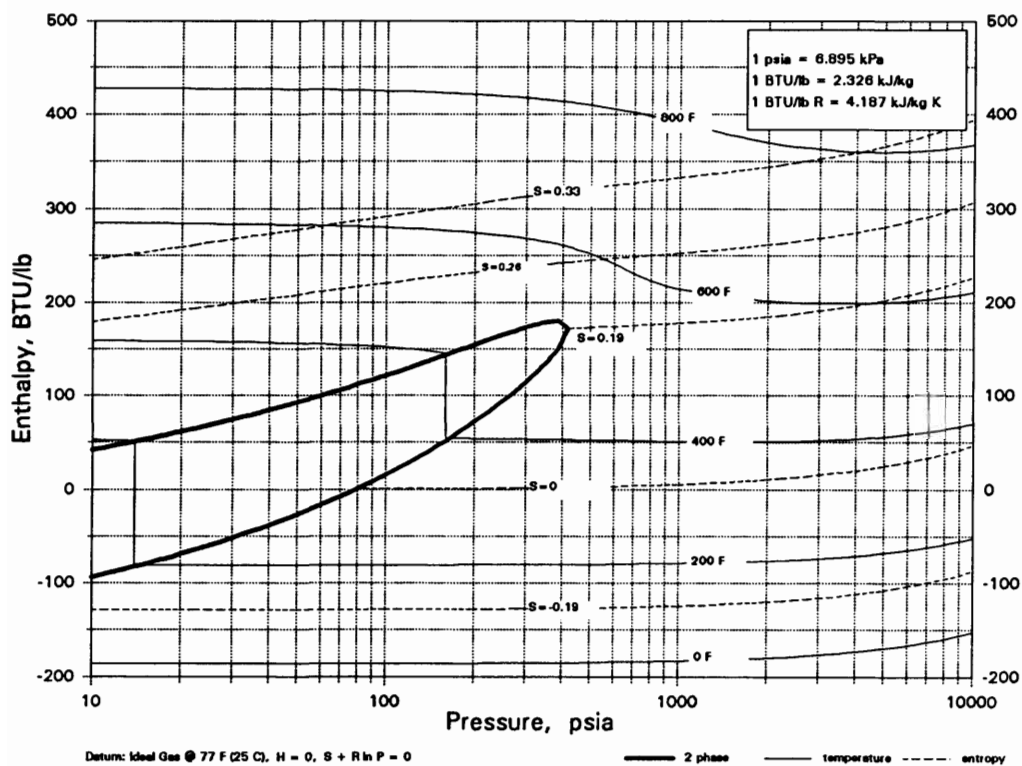
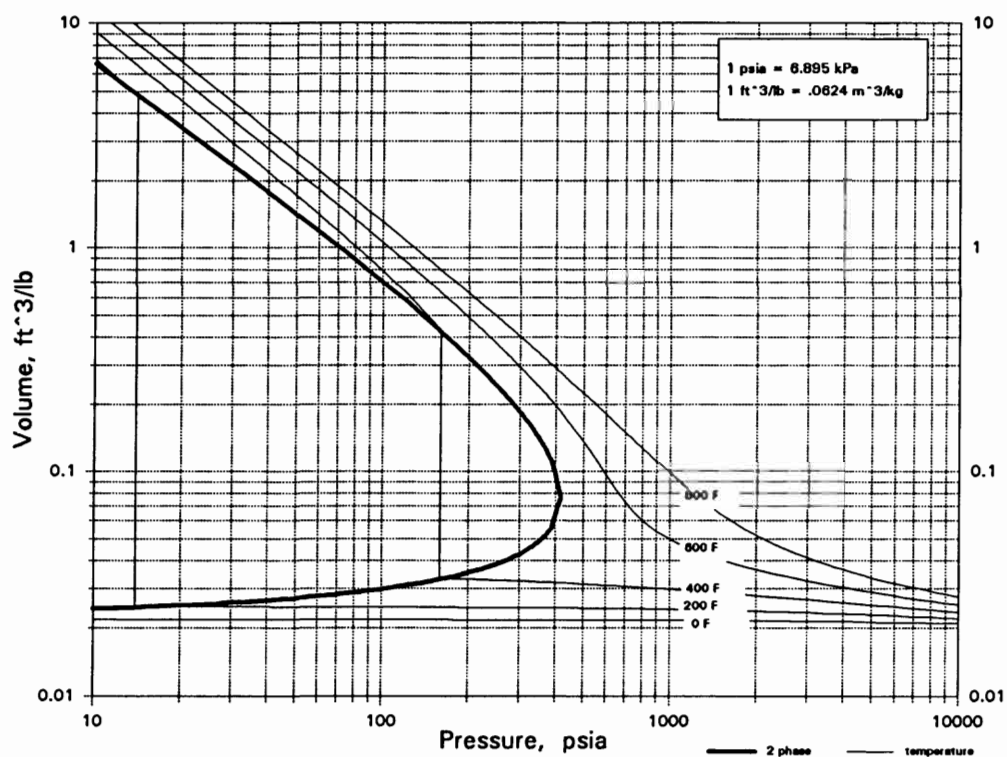
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3-3-DIMETHYLPENTANE



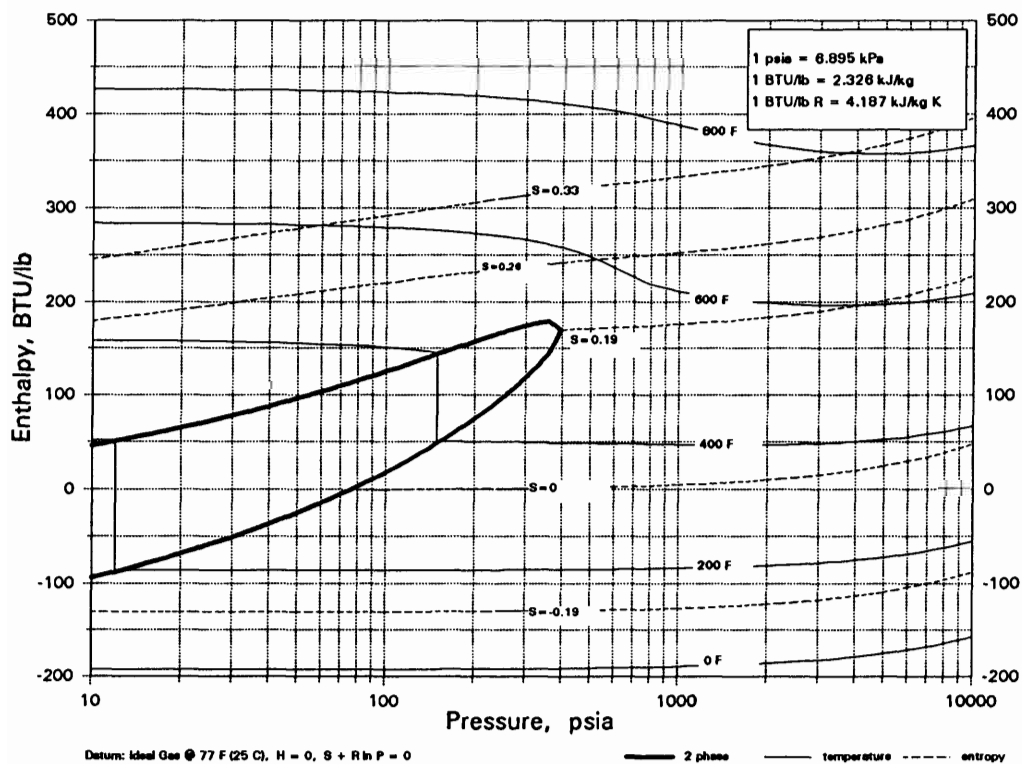
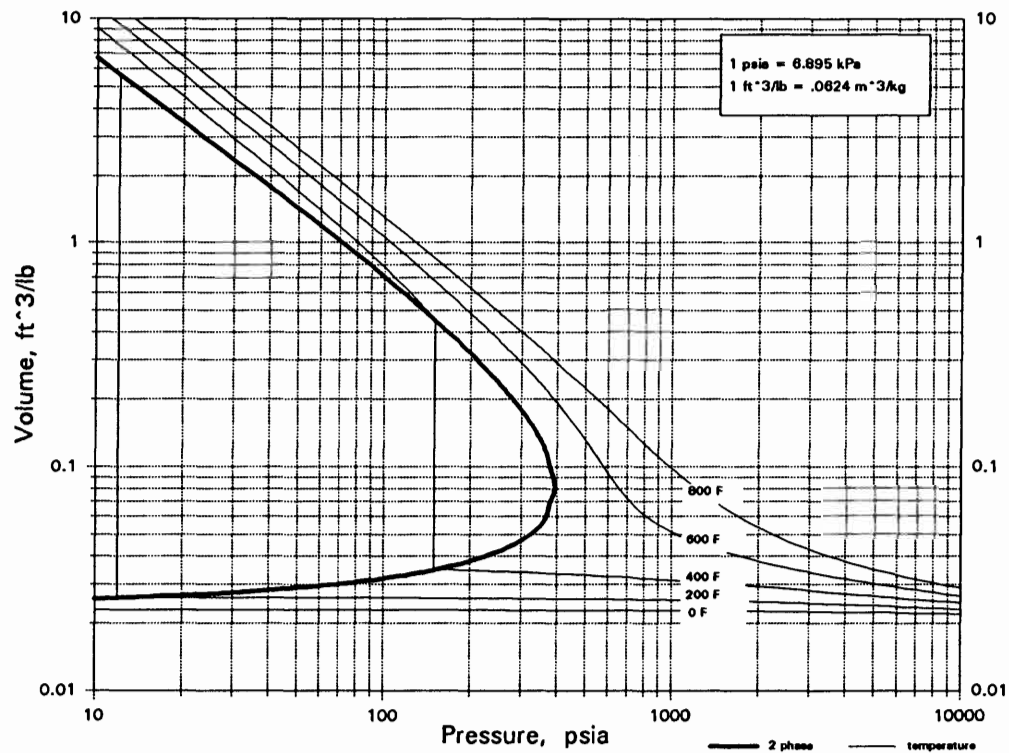
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3-ETHYLPENTANE



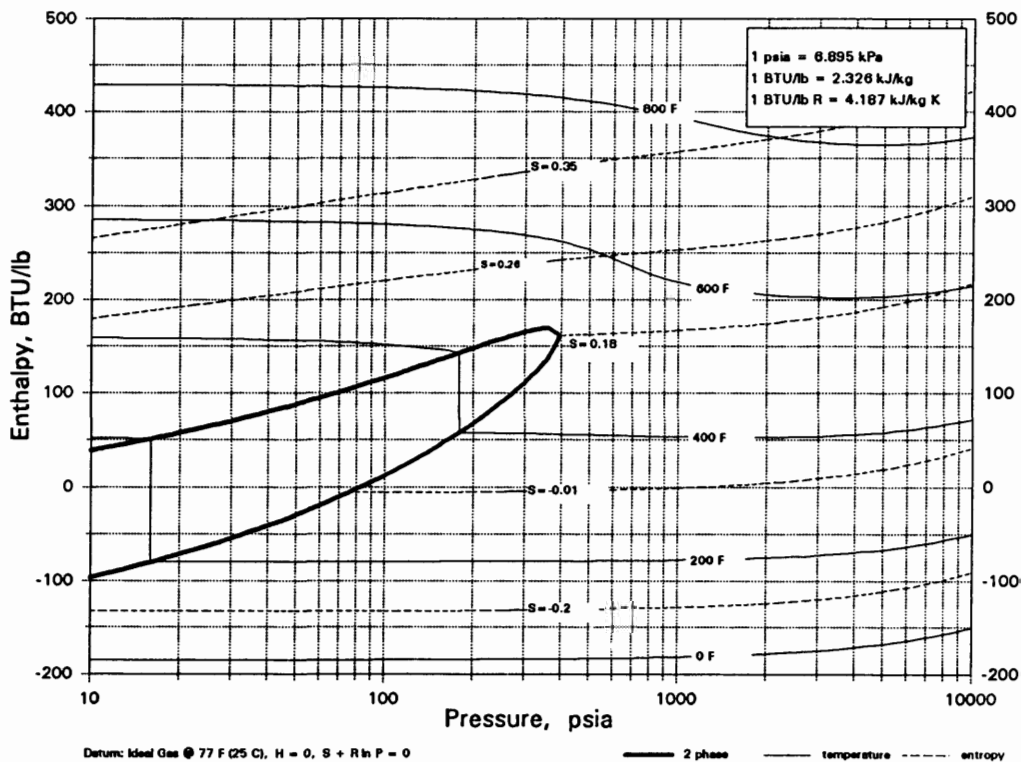
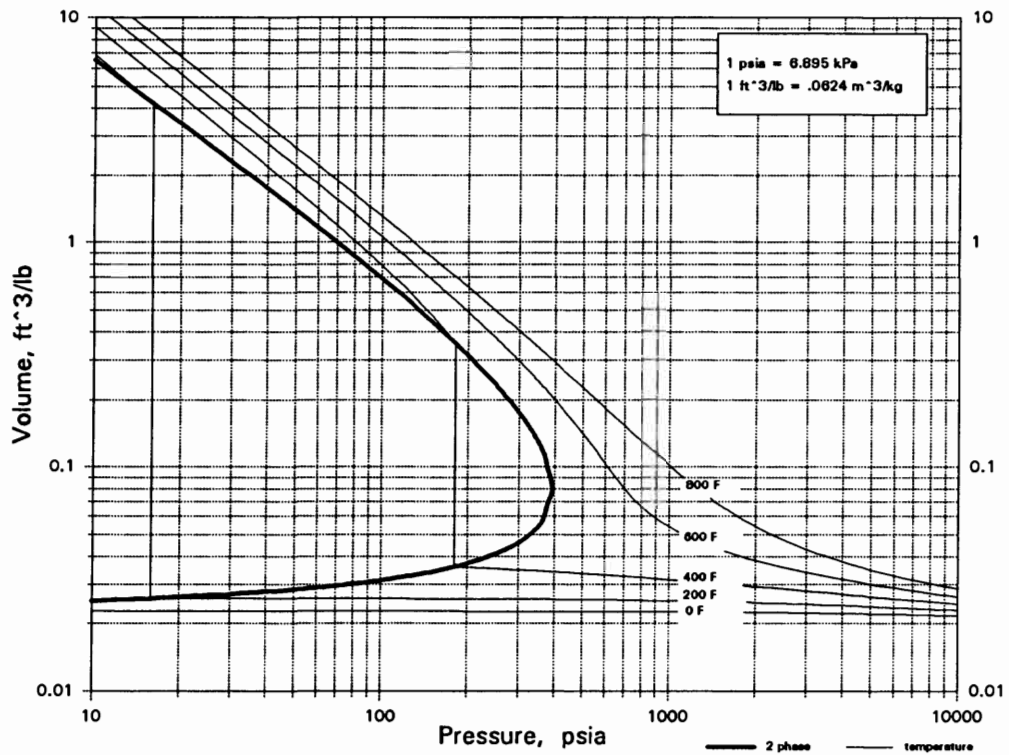
C7H16

n-HEPTANE



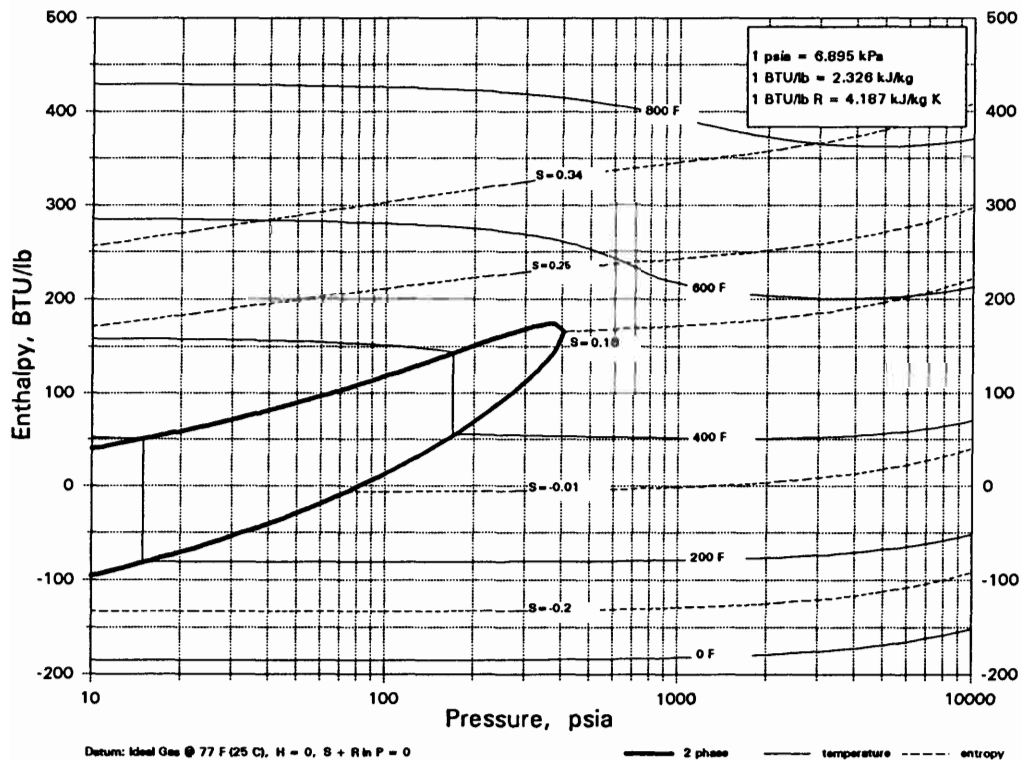
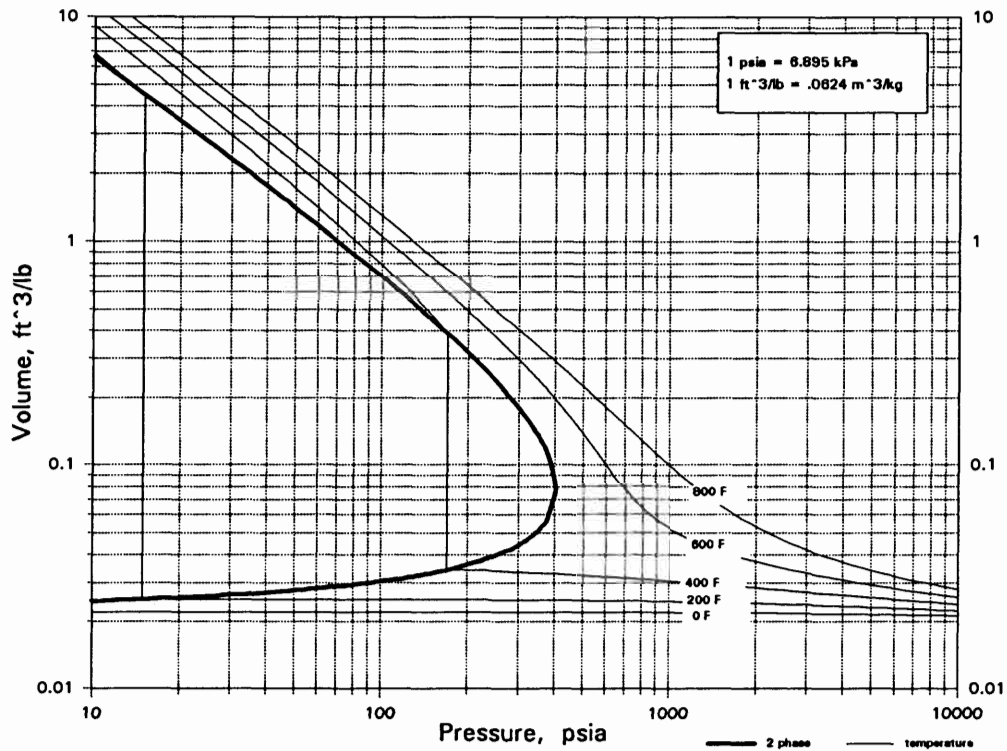
C7H16

2-METHYLHEXANE



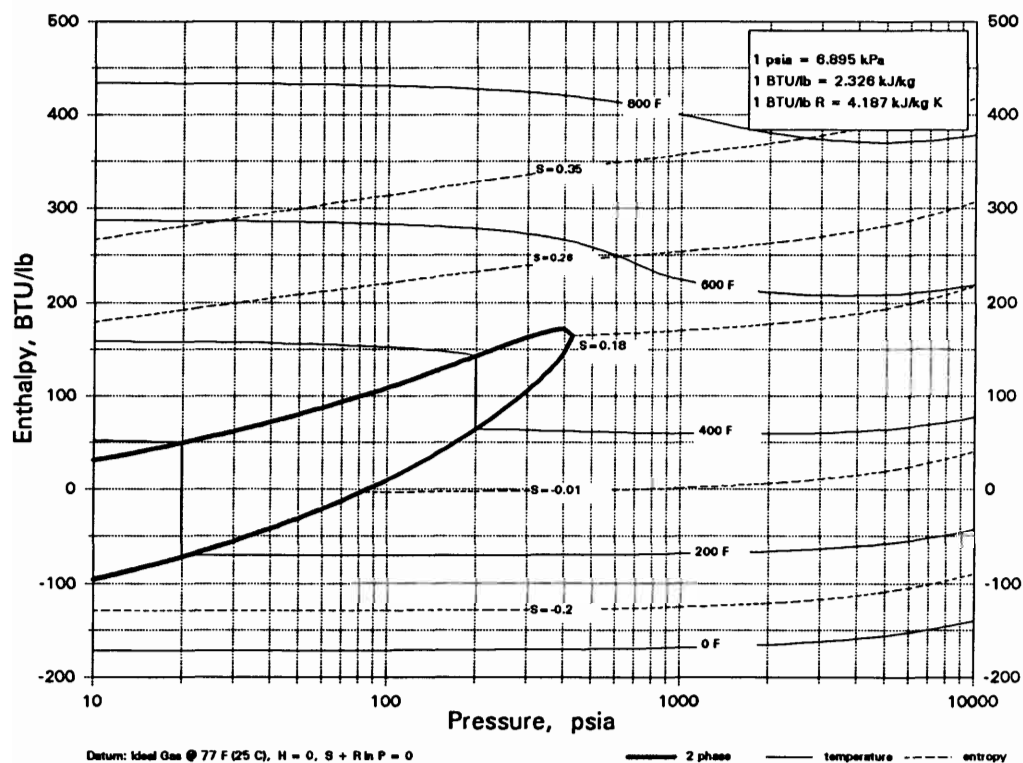
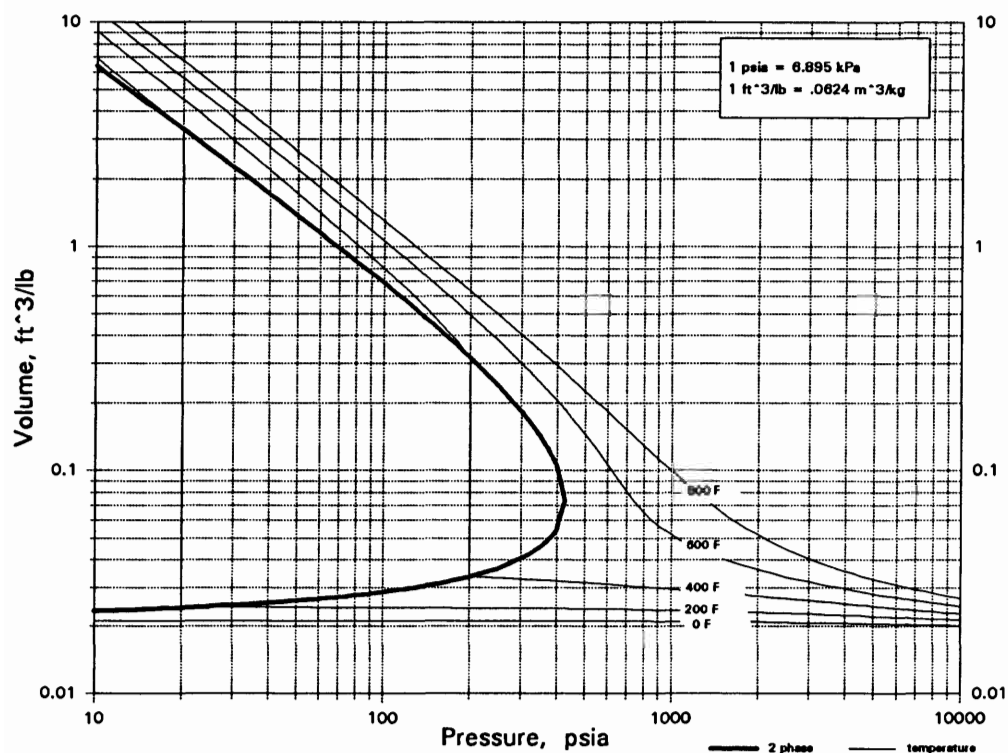
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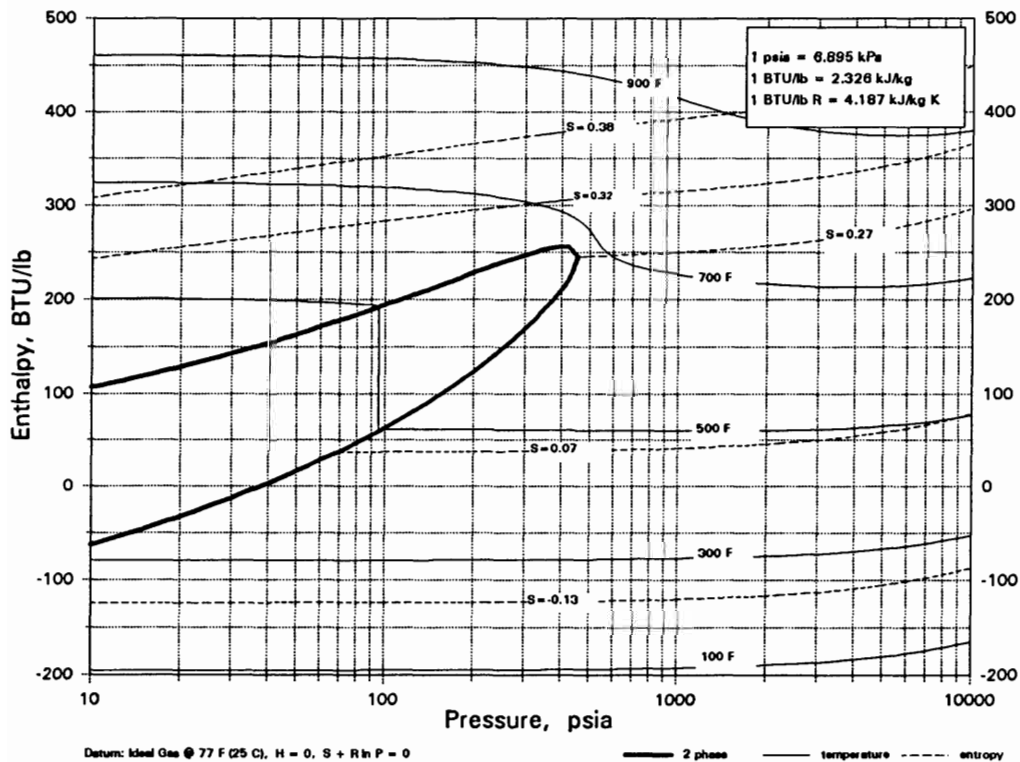
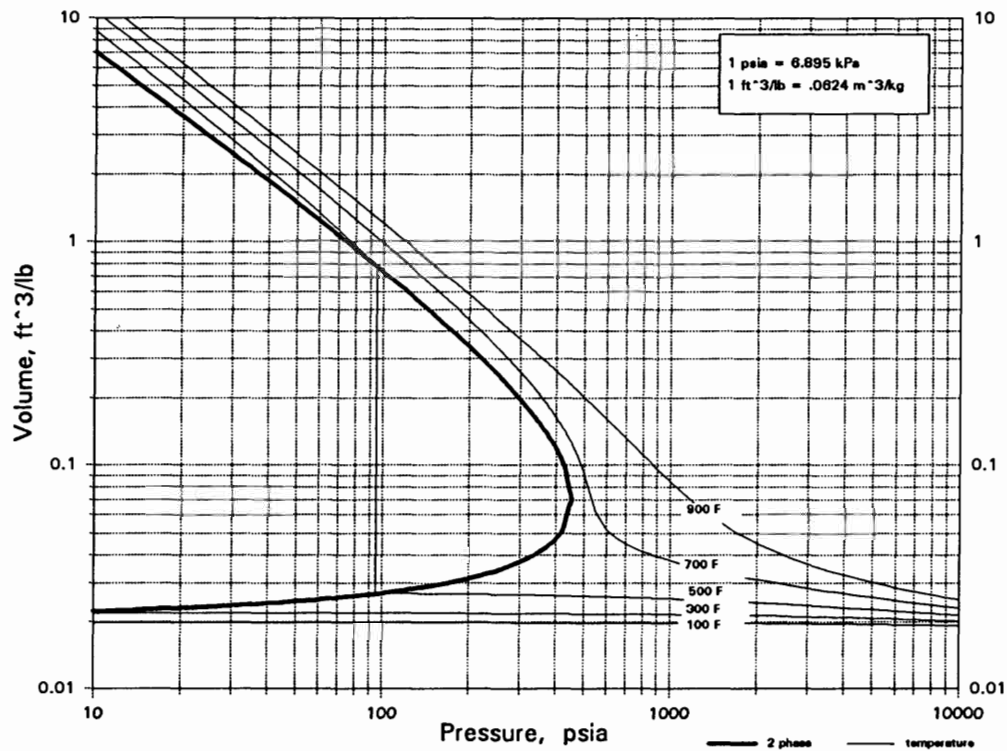
C7H16

2-2-3-TRIMETHYLBUTANE

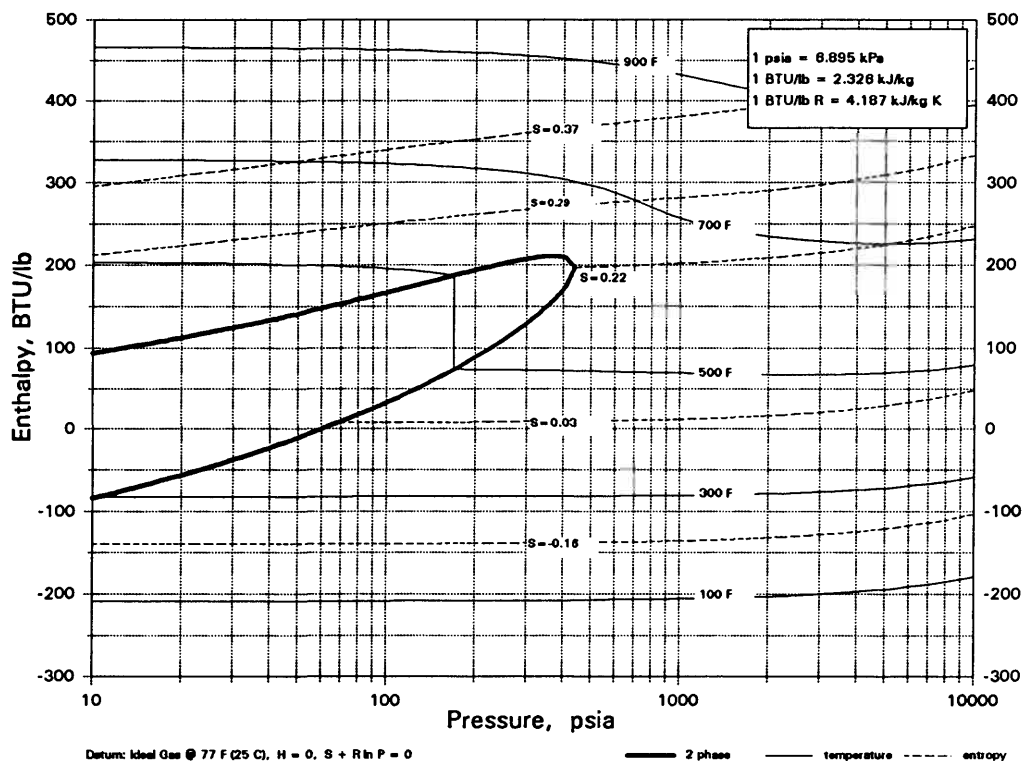
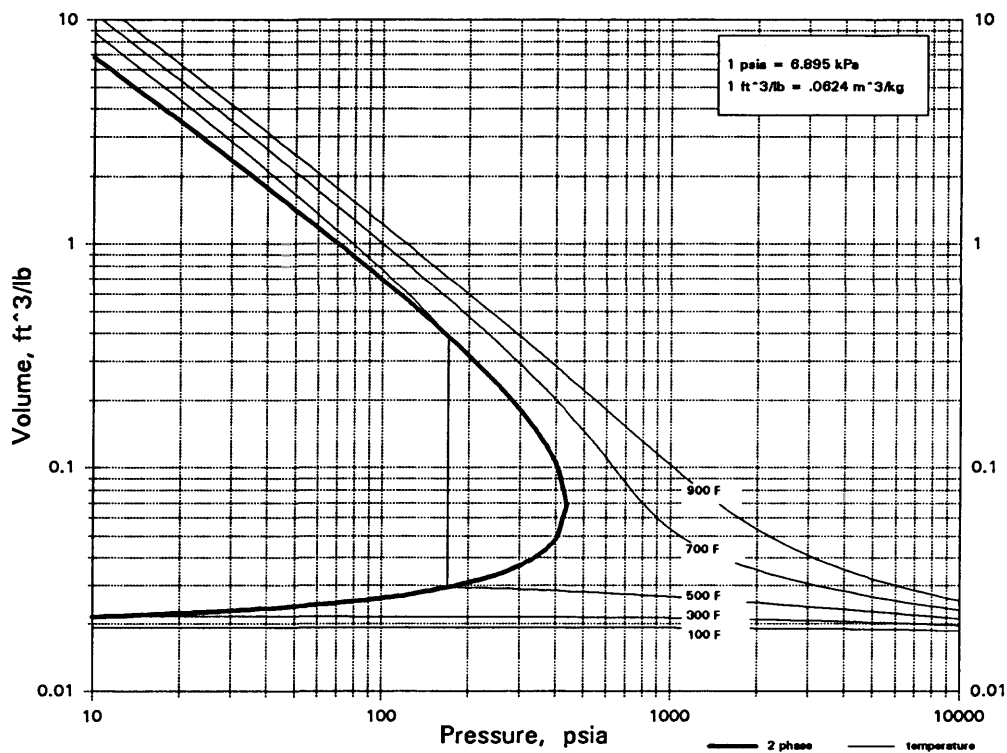


C7H16O

1-HEPTANOL

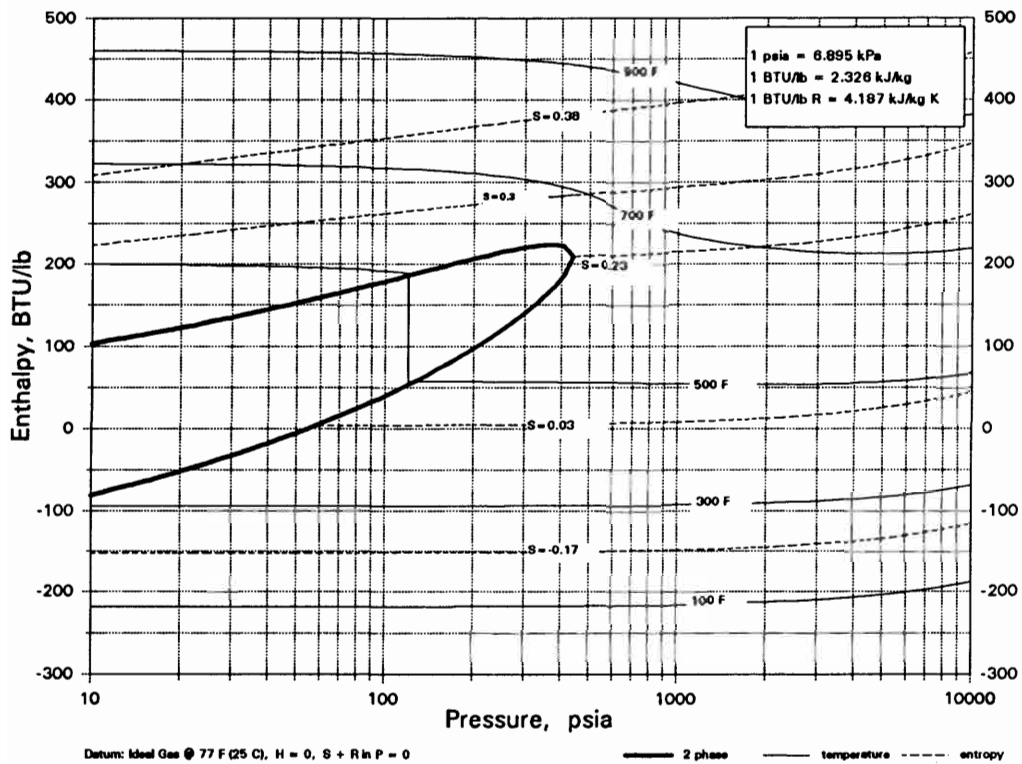
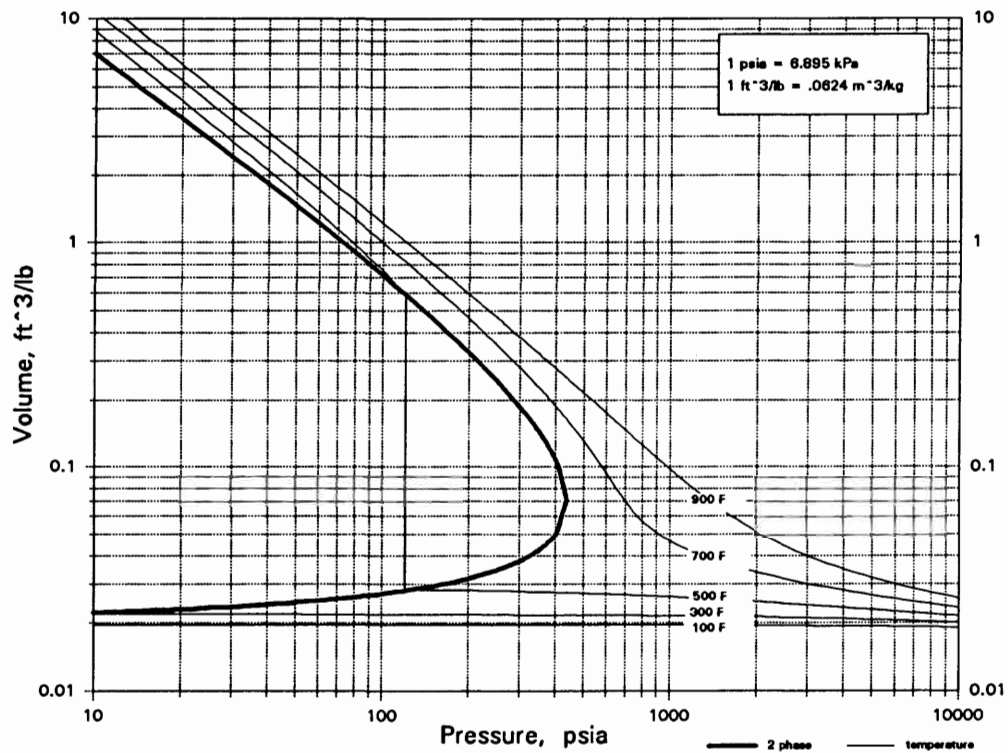


C7H16O
2-HEPTANOL



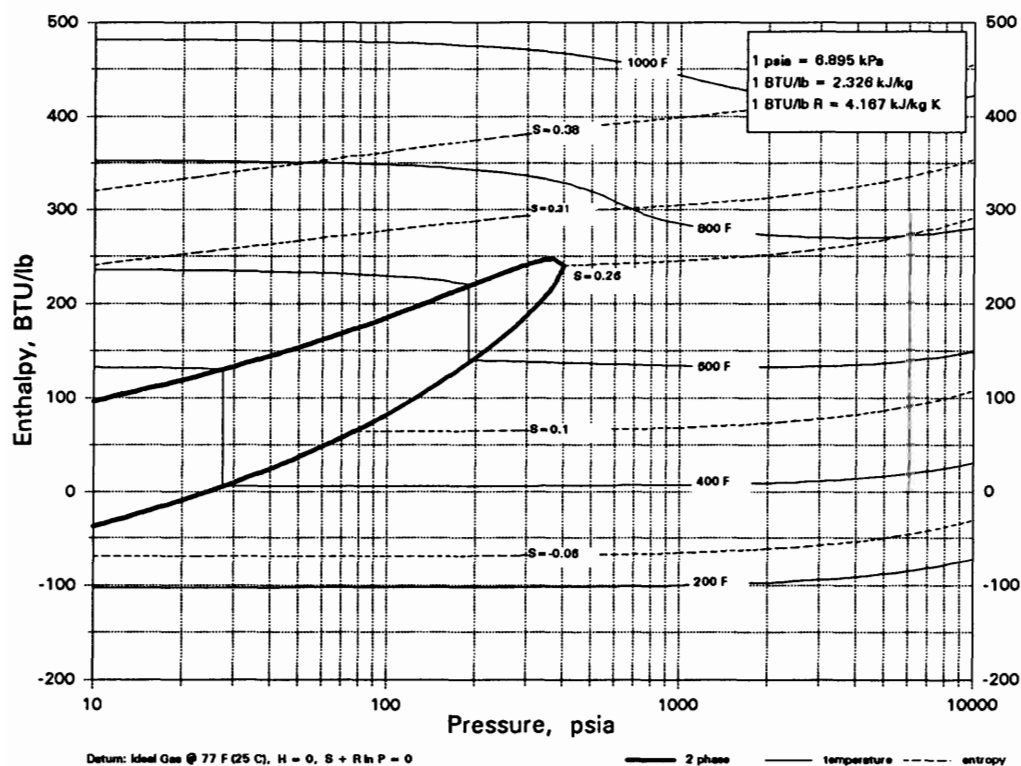
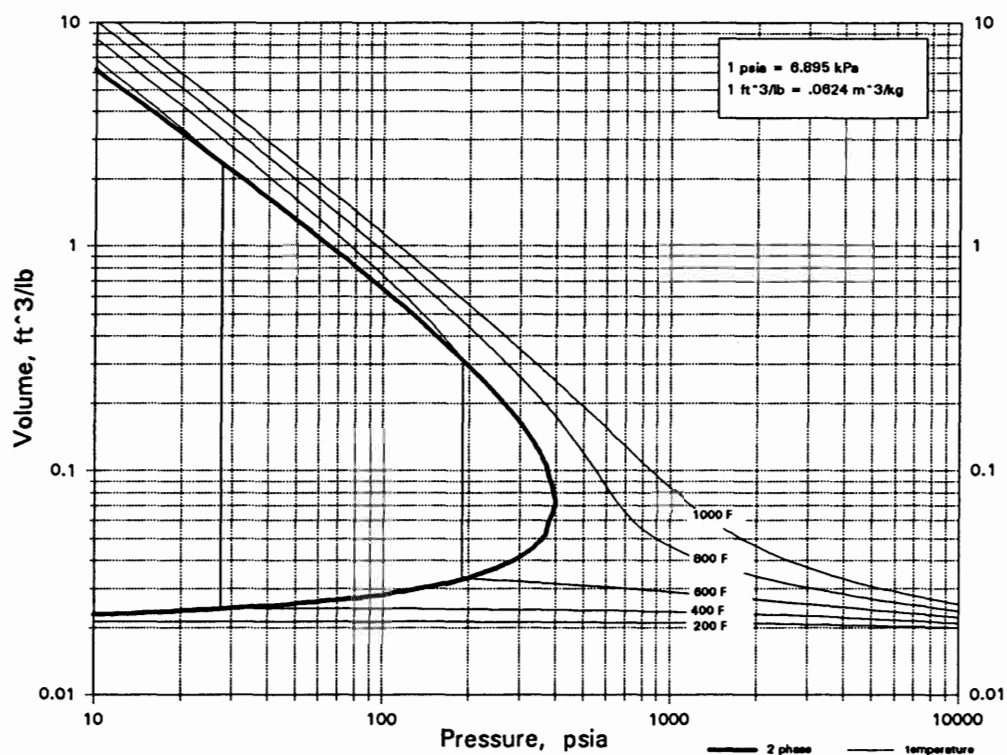
C7H16O

5-METHYL-1-HEXANOL



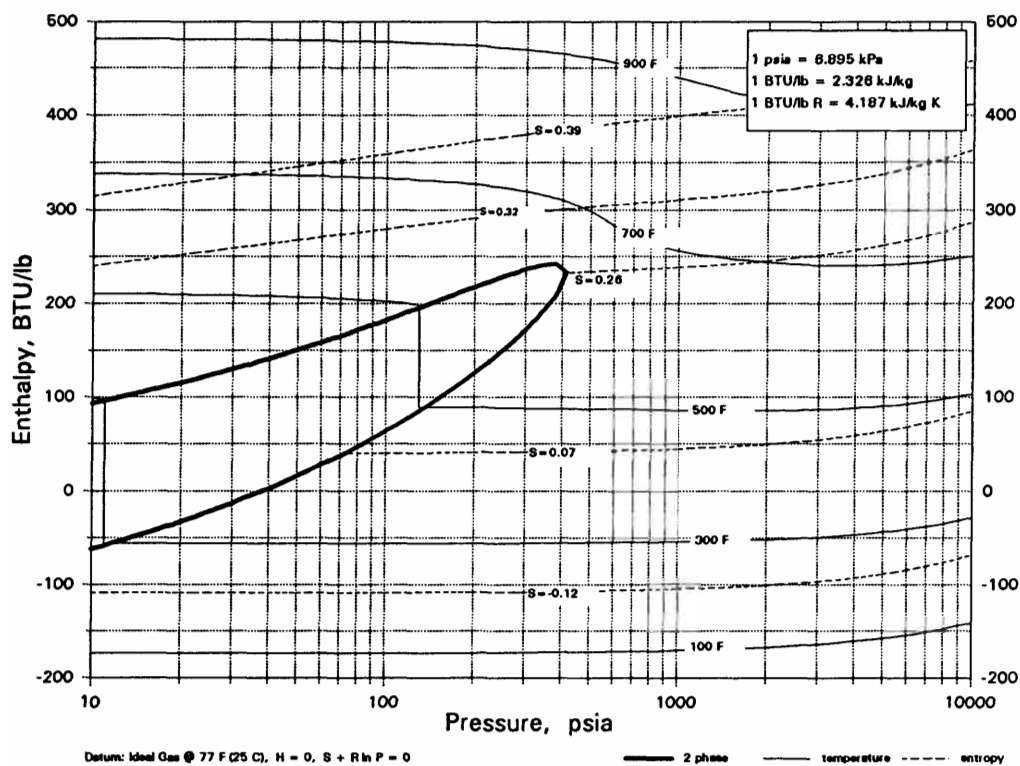
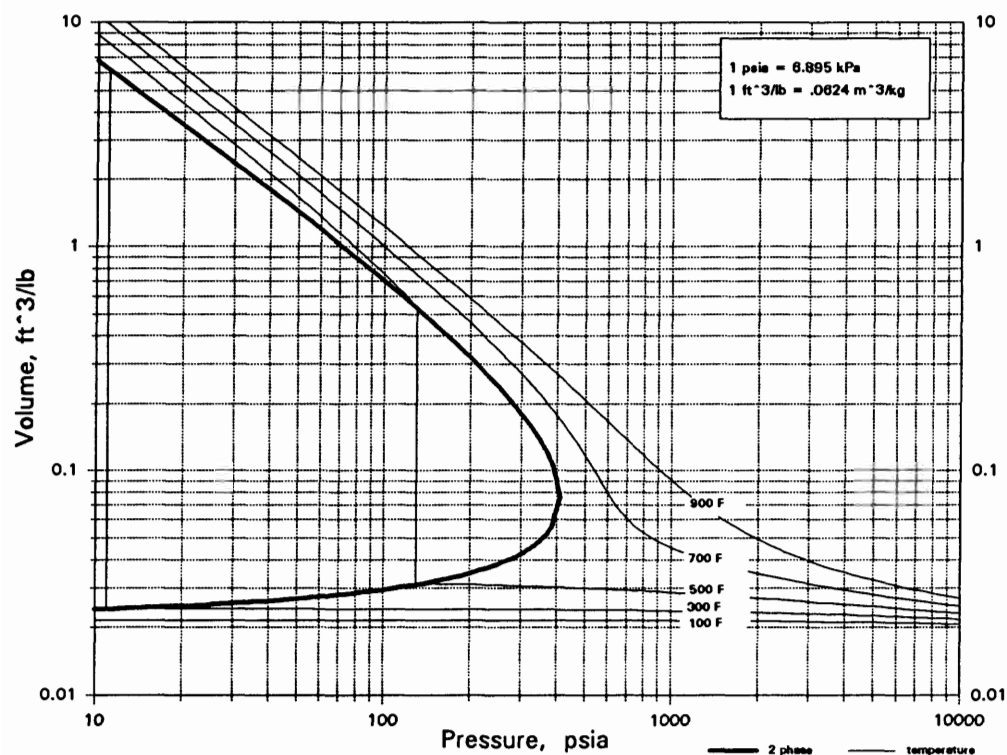
C7H16S

n-HEPTYL MERCAPTAN



C7H17N

1-AMINOHEPTANE



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Appendix A

Equations for Thermodynamic Properties

Enthalpy

$$H = H_{ref} + \int_{T_{ref}}^T C_p dT - \Delta H^{resid} \quad (1)$$

Entropy

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

Internal Energy

$$U = H - P V \quad (3)$$

Helmholtz Energy

$$A = U - T S \quad (4)$$

Gibbs Energy

$$G = H - T S \quad (5)$$

Parameters

$$C_p = \text{heat capacity of ideal gas} \quad (6)$$

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

$$T_{ref}, P_{ref} = \text{reference temperature, reference pressure} \quad (8)$$

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

Appendix B

Peng-Robinson Equation of State for Thermodynamic Properties

Equation of State

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

Volume

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

Compressibility Factor

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

Fugacity Coefficient

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

Residual Enthalpy

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

Residual Entropy

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

Parameters

$$a = a_c \alpha \quad (7)$$

$$a_c = 0.45724R^2T_c^2/P_c \quad (8)$$

$$b = 0.07780RT_c/P_c \quad (9)$$

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

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

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

$$A = aP/R^2T^2 = 0.45724\alpha P_x/T_x^2 = 0.45724 \frac{(P/P_c)}{(T/T_c)^2} \alpha \quad (13)$$

$$B = bP/RT = 0.07780P_x/T_x = 0.07780 \frac{(P/P_c)}{(T/T_c)} \quad (14)$$

$$D = -T \frac{da}{dT} = ma\sqrt{T_x/\alpha} \quad (15)$$

Appendix C

Examples for Thermodynamic Diagrams

Example 1 - Vessel Pressure

A vessel containing gaseous 1-pentene (C₅H₁₀) at 260 psia and 300 F is exposed to a fire in the process area. The temperature in the vessel is 700 F when the fire is extinguished. Estimate the final pressure in the vessel.

Since the vessel size does not change appreciably, this situation may be approximated by a constant volume process. Using the thermodynamic diagram, the initial volume is about 0.3 ft³/lb. At this same volume and final temperature, the pressure is:

$$\underline{P_{\text{final}} = 520 \text{ psia}}$$

Example 2 - Reactor Size

A batch reactor is to contain 2,000 lb of 1-pentene (C₅H₁₀) at 400 psia and 500 F. Estimate the reactor size.

Using the thermodynamic diagram, the volume is about 0.3 ft³/lb at these conditions. Substitution of this into the equation below for the reactor size provides:

$$\underline{\text{Reactor Size} = (2,000 \text{ lb}) (0.3 \text{ ft}^3/\text{lb}) = 600 \text{ ft}^3}$$

Example 3 - Process Vessel Size

A process vessel is to contain 500 lb of 1-pentene (C₅H₁₀) at 100 psia and 500 F. Estimate the process vessel size.

Using the thermodynamic diagram, the volume is about 1 ft³/lb at these conditions. Substitution of this into the equation below for the process vessel size provides:

$$\underline{\text{Vessel Size} = (500 \text{ lb}) (1 \text{ ft}^3/\text{lb}) = 500 \text{ ft}^3}$$

Example 4 - Heat Exchanger Duty

1-Pentene (C₅H₁₀, 30,000 lb/hr) at 1,000 psia and 100 F is heated to 500 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:

$$\begin{aligned} \underline{\text{Heat Exchanger Duty} = \text{mass flow} (H_2 - H_1) = (30,000 \text{ lb/hr})(145 - (-145)) \text{ BTU/lb}} \\ = \underline{8.7 \text{ million BTU/hr}} \end{aligned}$$

Example 5 - Compression

1-Pentene (C₅H₁₀, 20,000 lb/hr) at 50 psia and 300 F is compressed to 6,500 psia. Estimate the change in enthalpy for the compression assuming adiabatic and reversible conditions (constant entropy).

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

$$\begin{aligned}\text{Enthalpy Change} &= \text{mass flow } (H_2 - H_1) = (20,000 \text{ lb/hr})(200 - 100) \text{ BTU/lb} \\ &= \underline{2.0 \text{ million BTU/hr}}\end{aligned}$$

This change in enthalpy represents energy that is required to accomplish the compression under adiabatic 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-Pentene (C₅H₁₀, 30,000 lb/hr) at 2,000 psia and 700 F is expanded to 10 psia. Estimate the change in enthalpy for the expansion assuming adiabatic and reversible conditions (constant entropy).

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

$$\begin{aligned}\text{Enthalpy Change} &= \text{mass flow } (H_2 - H_1) = (30,000 \text{ lb/hr})(145 - 275) \text{ BTU/lb} \\ &= \underline{- 3.9 \text{ million BTU/hr}}\end{aligned}$$

This change in enthalpy represents energy that is available from the expansion under adiabatic 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 C₅ TO C₇ 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	C5Cl6	HEXACHLOROCYCLOPENTADIENE	272.771	284.49	512.15	746.00	30.10	526.0	0.5186	0.255	0.369
2	C5H4O2	FURFURAL	96.086	236.65	434.85	657.00	55.12	252.0	0.3813	0.254	0.444
3	C5H5N	PYRIDINE	79.101	231.53	388.41	619.95	56.34	254.0	0.3114	0.278	0.239
4	C5H6	CYCLOPENTADIENE	66.103	188.15	314.65	507.00	51.50	225.0	0.2938	0.275	0.212
5	C5H6	2-METHYL-1-BUTENE-3-YNE	66.103	160.15	305.40	492.00	43.80	248.0	0.2665	0.266	0.137
6	C5H6	1-PENTENE-3-YNE	66.103	---	332.40	520.00	44.00	256.0	0.2582	0.261	0.252
7	C5H6	1-PENTENE-4-YNE	66.103	---	315.65	503.00	44.00	256.0	0.2582	0.269	0.179
8	C5H6N2	GLUTARONITRILE	94.116	244.21	559.15	782.00	31.50	352.0	0.2674	0.171	0.603
9	C5H6O2	FURFURYL ALCOHOL	98.101	258.52	443.15	632.00	53.50	263.0	0.3730	0.268	0.736
10	C5H6O3	GLUTARIC ANHYDRIDE	114.101	328.00	562.69	838.00	58.00	275.0	0.4149	0.229	0.537
11	C5H6O4	CITRACONIC ACID	130.100	356.15	607.00	829.00	42.40	340.0	0.3826	0.209	0.927
12	C5H6O4	ITACONIC ACID	130.100	438.75	601.00	821.00	42.40	340.0	0.3826	0.211	0.925
13	C5H7N	N-METHYLPYRROLE	81.117	216.91	385.89	610.00	47.70	283.0	0.2866	0.266	0.213
14	C5H7NO2	ETHYL CYANOACETATE	113.116	250.65	479.15	679.00	33.40	358.0	0.3160	0.212	0.573
15	C5H8	CYCLOPENTENE	68.118	138.13	317.38	507.00	47.90	240.0	0.2838	0.273	0.195
16	C5H8	ISOPRENE	68.118	127.27	307.21	484.00	38.50	276.0	0.2468	0.264	0.158
17	C5H8	3-METHYL-1-2-BUTADIENE	68.118	159.53	314.00	490.00	38.30	291.0	0.2341	0.274	0.187
18	C5H8	1-2-PENTADIENE	68.118	135.89	318.01	500.00	38.00	276.0	0.2468	0.252	0.154
19	C5H8	cis-1-3-PENTADIENE	68.118	132.35	317.22	499.00	37.40	276.0	0.2468	0.249	0.147
20	C5H8	trans-1-3-PENTADIENE	68.118	185.71	315.17	500.00	37.40	276.0	0.2468	0.248	0.116
21	C5H8	1-4-PENTADIENE	68.118	124.86	299.11	479.00	37.40	303.0	0.2248	0.285	0.084
22	C5H8	2-3-PENTADIENE	68.118	147.50	321.40	497.00	38.00	295.0	0.2309	0.271	0.218
23	C5H8	1-PENTYNE	68.118	167.45	313.33	481.20	41.70	277.0	0.2459	0.289	0.290
24	C5H8	3-METHYL-1-BUTYNE	68.118	183.45	302.15	463.20	42.00	275.0	0.2477	0.300	0.308
25	C5H8N4O12	PENTAERYTHRITOL TETRANITRATE	316.138	413.65	543.00	676.00	22.40	731.0	0.4325	0.291	1.451
26	C5H8O	CYCLOPENTANONE	84.118	221.85	403.80	626.00	58.50	258.0	0.3260	0.290	0.388
27	C5H8O	METHYL ISOPROPENYL KETONE	84.118	219.55	371.15	566.00	38.90	302.0	0.2785	0.250	0.286
28	C5H8O2	ACETYLACETONE	100.117	249.65	413.55	602.00	39.60	323.0	0.3100	0.256	0.496
29	C5H8O2	ALLYL ACETATE	100.117	138.00	377.15	559.00	36.80	323.0	0.3100	0.256	0.388
30	C5H8O2	ETHYL ACRYLATE	100.117	201.95	372.65	553.00	36.80	323.0	0.3100	0.259	0.378
31	C5H8O2	METHYL METHACRYLATE	100.117	224.95	373.45	564.00	36.80	323.0	0.3100	0.253	0.317
32	C5H8O2	VINYL PROPIONATE	100.117	---	364.35	546.00	36.80	323.0	0.3100	0.262	0.336
33	C5H8O3	2-HYDROXYETHYL ACRYLATE	116.117	213.00	484.00	662.00	39.80	359.0	0.3234	0.260	0.864
34	C5H8O3	LEVULINIC ACID	116.117	308.15	518.95	723.00	40.20	343.0	0.3385	0.229	0.787
35	C5H8O3	METHYL ACETOACETATE	116.117	193.15	444.85	642.00	37.10	343.0	0.3385	0.238	0.513
36	C5H8O4	GLUTARIC ACID	132.116	370.65	595.54	807.00	40.40	363.0	0.3640	0.219	0.959
37	C5H9N	VALERONITRILE	83.133	176.95	414.45	603.00	32.60	331.0	0.2512	0.215	0.415
38	C5H9NO	n-BUTYL ISOCYANATE	99.133	---	388.15	568.00	34.40	360.0	0.2754	0.262	0.415
39	C5H9NO	N-METHYL-2-PYRROLIDONE	99.133	249.15	475.15	724.00	47.80	316.0	0.3137	0.251	0.358
40	C5H9NO4	L-GLUTAMIC ACID	147.131	497.15	670.00	886.00	41.34	383.3	0.3839	0.215	1.197
41	C5H10	CYCLOPENTANE	70.134	179.31	322.40	511.76	45.02	258.3	0.2715	0.273	0.194
42	C5H10	2-METHYL-1-BUTENE	70.134	135.58	304.30	465.00	34.00	292.0	0.2402	0.257	0.229
43	C5H10	2-METHYL-2-BUTENE	70.134	139.39	311.71	471.00	34.00	292.0	0.2402	0.254	0.277
44	C5H10	3-METHYL-1-BUTENE	70.134	104.66	293.21	450.37	35.16	302.1	0.2322	0.284	0.229
45	C5H10	1-PENTENE	70.134	107.93	303.11	464.78	35.29	296.0	0.2369	0.270	0.233
46	C5H10	cis-2-PENTENE	70.134	121.75	310.08	475.93	36.54	302.1	0.2322	0.279	0.241
47	C5H10	trans-2-PENTENE	70.134	132.89	309.49	475.37	36.54	302.1	0.2322	0.279	0.237
48	C5H10Cl2	1-5-DICHLOROPENTANE	141.040	200.35	453.15	663.00	31.90	422.0	0.3342	0.244	0.385
49	C5H10O	METHYL ISOPROPYL KETONE	86.134	181.15	367.55	553.00	38.50	310.0	0.2779	0.260	0.350
50	C5H10O	2-PENTANONE	86.134	196.29	373.46	561.08	36.94	301.0	0.2862	0.238	0.346
51	C5H10O	DIETHYL KETONE	86.134	234.18	375.14	560.95	37.39	336.0	0.2564	0.269	0.350
52	C5H10O	VALERALDEHYDE	86.134	182.00	376.15	554.00	35.00	316.0	0.2726	0.240	0.393
53	C5H10O2	n-BUTYL FORMATE	102.133	181.25	379.25	559.00	35.10	336.0	0.3040	0.254	0.384
54	C5H10O2	ETHYL PROPIONATE	102.133	199.25	372.25	546.00	33.62	345.0	0.2960	0.256	0.394
55	C5H10O2	ISOBUTYL FORMATE	102.133	177.35	371.22	551.35	38.81	352.0	0.2902	0.298	0.390
56	C5H10O2	ISOPROPYL ACETATE	102.133	199.75	361.65	538.00	35.80	336.0	0.3040	0.269	0.355
57	C5H10O2	n-PROPYL ACETATE	102.133	178.15	374.65	549.40	33.60	345.0	0.2960	0.254	0.394
58	C5H10O2	METHYL n-BUTYRATE	102.133	187.35	375.90	554.50	34.73	340.0	0.3004	0.256	0.381
59	C5H10O2	2-METHYLBUTYRIC ACID	102.133	---	450.15	643.00	38.90	347.0	0.2943	0.252	0.589
60	C5H10O2	ISOVALERIC ACID	102.133	243.85	448.25	634.00	38.90	336.0	0.3040	0.248	0.648
61	C5H10O2	VALERIC ACID	102.133	239.15	458.65	651.00	38.10	336.0	0.3040	0.237	0.627
62	C5H10O2	TETRAHYDROFURFURYL ALCOHOL	102.133	---	451.15	639.00	46.60	290.0	0.3522	0.254	0.703
63	C5H10O2S	3-METHYL SULFOLANE	134.199	273.65	549.15	817.00	42.40	353.0	0.3802	0.220	0.419
64	C5H10O3	DIETHYL CARBONATE	118.133	230.15	399.95	576.00	33.90	356.0	0.3318	0.252	0.485
65	C5H10O3	ETHYL LACTATE	118.133	247.15	427.65	588.00	38.60	354.0	0.3337	0.280	0.793

NO	FORMULA	NAME	MW g/mol	T _F K	T _B K	T _C K	P _C bar	V _G cm ³ /mol	ρ _C g/cm ³	Z _C	ω
66	C5H11Cl	1-CHLOROPENTANE	106.595	174.15	381.54	568.00	33.50	352.0	0.3028	0.250	0.334
67	C5H11N	N-METHYLPYRROLIDINE	85.149	183.15	352.30	550.00	42.00	298.0	0.2857	0.274	0.227
68	C5H11N	PIPERIDINE	85.149	262.65	379.55	594.05	46.51	308.0	0.2765	0.290	0.243
69	C5H11NO	tert-BUTYLFORMAMIDE	101.148	289.15	475.15	692.00	35.60	383.0	0.2641	0.237	0.449
70	C5H12	ISOPENTANE	72.150	113.25	300.99	460.43	33.81	305.8	0.2359	0.270	0.228
71	C5H12	NEOPENTANE	72.150	256.58	282.65	433.78	31.99	303.6	0.2377	0.269	0.196
72	C5H12	n-PENTANE	72.150	143.42	309.22	469.65	33.69	312.3	0.2310	0.269	0.249
73	C5H12O	2-2-DIMETHYL-1-PROPANOL	88.150	327.15	386.25	550.00	38.80	327.0	0.2696	0.277	0.604
74	C5H12O	2-METHYL-1-BUTANOL	88.150	---	401.85	565.00	38.80	327.0	0.2696	0.270	0.678
75	C5H12O	2-METHYL-2-BUTANOL	88.150	264.35	375.15	545.15	38.80	327.0	0.2696	0.280	0.483
76	C5H12O	3-METHYL-1-BUTANOL	88.150	155.95	404.35	579.45	38.80	327.0	0.2696	0.263	0.556
77	C5H12O	3-METHYL-2-BUTANOL	88.150	---	384.65	574.00	39.60	327.0	0.2696	0.271	0.351
78	C5H12O	1-PENTANOL	88.150	195.56	410.95	586.15	38.80	326.0	0.2704	0.260	0.594
79	C5H12O	2-PENTANOL	88.150	200.00	392.15	552.00	38.80	327.0	0.2696	0.276	0.675
80	C5H12O	3-PENTANOL	88.150	204.15	388.45	547.00	38.80	327.0	0.2696	0.279	0.675
81	C5H12O	METHYL sec-BUTYL ETHER	88.150	---	332.15	498.00	34.10	329.0	0.2679	0.271	0.306
82	C5H12O	METHYL tert-BUTYL ETHER	88.150	164.55	328.35	497.10	34.30	329.0	0.2679	0.273	0.267
83	C5H12O	METHYL ISOBUTYL ETHER	88.150	---	331.70	497.00	34.10	329.0	0.2679	0.272	0.310
84	C5H12O	ETHYL PROPYL ETHER	88.150	145.65	337.01	500.23	33.70	339.0	0.2600	0.275	0.346
85	C5H12O2	ETHYLENE GLYCOL MONOPROPYL ETHER	104.149	183.15	424.50	582.00	36.70	347.0	0.3001	0.263	0.783
86	C5H12O2	NEOPENTYL GLYCOL	104.149	400.00	483.00	643.00	42.40	345.0	0.3019	0.274	1.143
87	C5H12O2	1-5-PENTANEDIOL	104.149	257.15	512.15	673.00	41.50	345.0	0.3019	0.256	1.220
88	C5H12O3	2-(2-METHOXYETHOXY)ETHANOL	120.148	197.15	466.75	630.00	35.40	367.0	0.3274	0.248	0.870
89	C5H12O4	PENTAERYTHRITOL	136.148	534.15	631.00	780.00	47.80	381.0	0.3573	0.281	2.120
90	C5H12S	n-PENTYL MERCAPTAN	104.216	197.45	399.79	598.00	34.70	359.0	0.2903	0.251	0.321
91	C5H13N	n-PENTYLAMINE	87.165	218.15	377.65	555.00	35.80	365.0	0.2388	0.283	0.407
92	C5H13NO2	METHYL DIETHANOLAMINE	119.164	252.15	520.15	678.00	38.80	401.0	0.2972	0.276	1.302
93	C6Cl6	HEXACHLOROBENZENE	284.782	501.70	582.55	825.00	28.50	526.0	0.5414	0.219	0.497
94	C6F6	HEXAFLUOROBENZENE	186.056	278.25	353.41	516.73	32.73	335.0	0.5554	0.255	0.395
95	C6H3ClN2O4	1-CHLORO-2-4-DINITROBENZENE	202.554	326.55	588.00	813.77	34.90	478.0	0.4238	0.247	0.732
96	C6H3Cl2N2O2	1-2-DICHLORO-4-NITROBENZENE	192.001	315.65	529.00	758.00	36.00	436.0	0.4404	0.249	0.539
97	C6H3Cl3	1-2-4-TRICHLOROBENZENE	181.448	290.15	486.15	725.00	37.20	395.0	0.4594	0.244	0.358
98	C6H3N3O6	1-3-5-TRINITROBENZENE	213.106	398.40	748.00	1005.00	33.90	520.0	0.4098	0.211	0.808
99	C6H4Br2	m-DIBROMOBENZENE	235.906	266.25	491.15	761.00	46.60	372.0	0.6342	0.274	0.293
100	C6H4ClNO2	m-CHLORONITROBENZENE	157.556	317.65	508.75	742.00	39.80	432.0	0.3647	0.279	0.489
101	C6H4ClNO2	o-CHLORONITROBENZENE	157.556	306.15	519.00	757.00	39.80	432.0	0.3647	0.273	0.483
102	C6H4ClNO2	p-CHLORONITROBENZENE	157.556	356.65	515.15	751.00	39.80	432.0	0.3647	0.275	0.491
103	C6H4Cl2	m-DICHLOROBENZENE	147.003	248.39	446.23	683.95	40.70	351.0	0.4188	0.251	0.279
104	C6H4Cl2	o-DICHLOROBENZENE	147.003	256.15	453.57	705.00	40.70	351.0	0.4188	0.244	0.219
105	C6H4Cl2	p-DICHLOROBENZENE	147.003	326.14	447.21	684.75	40.70	351.0	0.4188	0.251	0.285
106	C6H4N2O4	m-DINITROBENZENE	168.109	364.00	573.00	805.00	38.50	434.0	0.3873	0.250	0.682
107	C6H4N2O4	o-DINITROBENZENE	168.109	390.08	592.00	831.00	38.50	434.0	0.3873	0.242	0.687
108	C6H4N2O4	p-DINITROBENZENE	168.109	446.60	572.00	803.00	38.50	434.0	0.3873	0.250	0.686
109	C6H5Br	BROMOBENZENE	157.010	242.43	429.24	670.15	45.19	324.0	0.4846	0.263	0.251
110	C6H5Cl	MONOCHLOROBENZENE	112.558	227.95	404.87	632.35	45.19	308.0	0.3654	0.265	0.251
111	C6H5ClO	m-CHLOROPHENOL	128.558	306.00	487.00	729.00	53.20	320.0	0.4017	0.281	0.486
112	C6H5ClO	o-CHLOROPHENOL	128.558	282.00	447.53	675.00	50.00	325.0	0.3956	0.290	0.437
113	C6H5ClO	p-CHLOROPHENOL	128.558	316.00	493.11	738.00	53.20	325.0	0.3956	0.282	0.485
114	C6H5Cl2N	3-4-DICHLOROANILINE	162.018	344.65	545.00	800.00	41.10	409.0	0.3961	0.253	0.468
115	C6H5F	FLUOROBENZENE	96.104	230.94	357.88	560.09	45.51	269.0	0.3573	0.263	0.247
116	C6H5I	IODOBENZENE	204.010	241.83	461.60	721.15	45.19	351.0	0.5812	0.265	0.247
117	C6H5NO2	NITROBENZENE	123.111	278.91	483.95	719.00	44.00	349.0	0.3528	0.257	0.448
118	C6H6	BENZENE	78.114	278.68	353.24	562.16	48.98	258.9	0.3017	0.271	0.211
119	C6H6ClN	m-CHLOROANILINE	127.573	262.75	501.65	751.00	45.90	364.0	0.3505	0.268	0.420
120	C6H6ClN	o-CHLOROANILINE	127.573	481.99	481.99	722.00	45.90	364.0	0.3505	0.278	0.425
121	C6H6ClN	p-CHLOROANILINE	127.573	343.05	503.65	754.00	45.90	364.0	0.3505	0.267	0.421
122	C6H6N2	cis-DICYANO-1-BUTENE	106.127	249.00	501.00	691.00	29.50	392.0	0.2707	0.201	0.672
123	C6H6N2	trans-DICYANO-1-BUTENE	106.127	260.00	499.00	689.00	29.50	392.0	0.2707	0.202	0.664
124	C6H6N2	1-4-DICYANO-2-BUTENE	106.127	349.00	547.00	755.00	29.50	426.0	0.2491	0.200	0.667
125	C6H6N2O2	m-NITROANILINE	138.126	387.15	579.00	815.00	44.20	406.0	0.3402	0.265	0.740
126	C6H6N2O2	o-NITROANILINE	138.126	344.65	558.00	784.00	44.20	406.0	0.3402	0.275	0.741
127	C6H6N2O2	p-NITROANILINE	138.126	420.65	609.15	851.00	44.20	406.0	0.3402	0.254	0.782
128	C6H6O	PHENOL	94.113	314.06	454.99	694.25	61.30	229.0	0.4110	0.243	0.426
129	C6H6O2	1-2-BENZENEDIOL	110.112	377.60	518.65	764.00	74.90	300.0	0.3670	0.354	0.701
130	C6H6O2	1-3-BENZENEDIOL	110.112	382.00	549.65	810.00	74.90	300.0	0.3670	0.334	0.677
131	C6H6O2	p-HYDROQUINONE	110.112	444.65	558.15	822.00	74.50	300.0	0.3670	0.327	0.686
132	C6H6O3	1-2-3-BENZENETRIOL	126.112	407.00	581.85	830.00	88.10	318.0	0.3966	0.406	0.945
133	C6H6S	PHENYL MERCAPTAN	110.180	258.26	442.29	689.00	47.40	315.0	0.3498	0.261	0.263
134	C6H7N	ANILINE	93.128	267.13	457.60	699.00	53.09	270.0	0.3449	0.247	0.404
135	C6H7N	2-METHYLPYRIDINE	93.128	206.44	402.55	621.00	43.80	320.0	0.2910	0.271	0.278
136	C6H7N	3-METHYLPYRIDINE	93.128	255.01	417.29	645.00	43.80	320.0	0.2910	0.261	0.271
137	C6H7N	4-METHYLPYRIDINE	93.128	276.73	418.50	646.15	46.61	325.6	0.2860	0.283	0.302
138	C6H8	1-3-CYCLOHEXADIENE	80.130	161.00	353.49	558.00	47.30	277.0	0.2893	0.282	0.231
139	C6H8	METHYLCYCLOPENTADIENE	80.130	---	345.93	541.00	44.30	279.0	0.2872	0.275	0.238
140	C6H8N2	ADIPONITRILE	108.143	275.64	568.15	781.00	28.30	406.0	0.2664	0.177	0.672
141	C6H8N2	METHYLGUTARONITRILE	108.143	228.15	536.15	742.00	28.80	404.0	0.2677	0.189	0.638

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
142	C6H8N2	m-PHENYLENEDIAMINE	108.143	334.00	560.00	824.00	51.80	377.0	0.2869	0.285	0.543
143	C6H8N2	o-PHENYLENEDIAMINE	108.143	376.95	525.00	781.00	51.80	315.0	0.3433	0.251	0.494
144	C6H8N2	p-PHENYLENEDIAMINE	108.143	413.00	540.00	796.00	51.80	317.0	0.3411	0.248	0.539
145	C6H8N2	PHENYLHYDRAZINE	108.143	292.35	516.65	761.00	49.10	418.0	0.2587	0.324	0.535
146	C6H8N2O	BIS(CYANOETHYL)ETHER	124.142	246.85	579.00	783.00	28.30	377.0	0.3293	0.164	0.782
147	C6H8O4	DIMETHYL MALEATE	144.127	254.15	478.15	675.00	32.20	403.0	0.3576	0.231	0.562
148	C6H8O6	ASCORBIC ACID	176.126	465.15	637.00	783.00	52.90	339.0	0.5195	0.275	2.389
149	C6H8O7	CITRIC ACID	192.125	426.15	659.00	822.00	37.98	419.7	0.4578	0.233	1.857
150	C6H10	CYCLOHEXENE	82.145	169.67	356.12	560.40	43.50	291.0	0.2823	0.272	0.214
151	C6H10	2-3-DIMETHYL-1-3-BUTADIENE	82.145	197.15	341.93	526.00	35.20	315.0	0.2608	0.254	0.214
152	C6H10	1-5-HEXADIENE	82.145	132.47	332.61	507.00	33.50	339.0	0.2423	0.269	0.232
153	C6H10	cis-trans-2-4-HEXADIENE	82.145	177.05	356.65	538.00	33.50	331.0	0.2482	0.248	0.275
154	C6H10	trans-trans-2-4-HEXADIENE	82.145	228.25	355.05	535.00	33.50	331.0	0.2482	0.249	0.282
155	C6H10	1-HEXYNE	82.145	141.25	344.48	516.20	36.20	322.0	0.2551	0.272	0.333
156	C6H10	2-HEXYNE	82.145	183.65	357.67	549.00	35.30	331.0	0.2482	0.256	0.221
157	C6H10	3-HEXYNE	82.145	170.05	354.35	544.00	35.30	331.0	0.2482	0.258	0.218
158	C6H10O	CYCLOHEXANONE	98.145	242.00	428.90	629.15	38.50	311.0	0.3156	0.229	0.450
159	C6H10O	MESITYL OXIDE	98.145	220.15	402.95	600.00	34.10	355.0	0.2765	0.243	0.327
160	C6H10O2	epsilon-CAPROLACTONE	114.144	271.85	514.00	771.00	46.30	352.0	0.3243	0.254	0.442
161	C6H10O2	ETHYL METHACRYLATE	114.144	---	390.15	577.00	32.50	375.0	0.3044	0.254	0.344
162	C6H10O2	n-PROPYL ACRYLATE	114.144	---	392.15	569.00	32.50	376.0	0.3036	0.258	0.434
163	C6H10O3	ETHYLACETOACETATE	130.144	234.15	453.95	643.00	32.70	391.0	0.3328	0.239	0.561
164	C6H10O3	PROPIONIC ANHYDRIDE	130.144	228.15	442.15	618.00	33.40	396.0	0.3286	0.257	0.618
165	C6H10O4	ADIPIC ACID	146.143	425.50	611.00	809.00	35.30	400.0	0.3654	0.210	1.054
166	C6H10O4	DIETHYL OXALATE	146.143	232.55	458.85	646.00	30.90	416.0	0.3513	0.239	0.568
167	C6H10O4	ETHYLENE GLYCOL DIACETATE	146.143	242.15	463.65	653.00	30.90	416.0	0.3513	0.237	0.560
168	C6H10O4	ETHYLIDENE DIACETATE	146.143	292.00	442.15	635.00	32.60	406.0	0.3600	0.251	0.478
169	C6H11N	HEXANENITRILE	97.160	192.85	436.75	622.05	29.20	384.0	0.2530	0.217	0.474
170	C6H11NO	epsilon-CAPROLACTAM	113.159	342.36	543.15	806.00	47.70	356.0	0.3179	0.253	0.477
171	C6H11NO	CYCLOHEXANONE OXIME	113.159	363.15	481.15	715.00	46.90	369.0	0.3067	0.291	0.462
172	C6H12	CYCLOHEXANE	84.161	279.69	353.87	553.54	40.75	307.9	0.2734	0.273	0.212
173	C6H12	2-3-DIMETHYL-1-BUTENE	84.161	115.89	328.76	500.00	32.20	349.0	0.2411	0.270	0.227
174	C6H12	2-3-DIMETHYL-2-BUTENE	84.161	198.82	346.35	524.00	31.60	372.0	0.2262	0.270	0.233
175	C6H12	3-3-DIMETHYL-1-BUTENE	84.161	157.95	314.40	480.00	32.90	333.0	0.2527	0.275	0.226
176	C6H12	2-ETHYL-1-BUTENE	84.161	141.61	337.82	512.00	31.60	364.0	0.2312	0.270	0.228
177	C6H12	1-HEXENE	84.161	133.39	336.63	504.03	31.40	354.0	0.2377	0.265	0.280
178	C6H12	cis-2-HEXENE	84.161	132.00	342.03	513.00	31.60	359.0	0.2344	0.266	0.272
179	C6H12	trans-2-HEXENE	84.161	140.17	341.02	513.00	31.60	360.0	0.2338	0.267	0.261
180	C6H12	cis-3-HEXENE	84.161	135.33	339.60	509.00	31.70	351.0	0.2398	0.263	0.279
181	C6H12	trans-3-HEXENE	84.161	159.73	340.24	509.00	31.70	351.0	0.2398	0.263	0.285
182	C6H12	METHYLCYCLOPENTANE	84.161	130.73	344.96	532.79	37.85	318.9	0.2639	0.272	0.230
183	C6H12	2-METHYL-1-PENTENE	84.161	137.42	335.25	507.00	31.60	359.0	0.2344	0.269	0.241
184	C6H12	2-METHYL-2-PENTENE	84.161	138.07	340.45	514.00	31.60	363.0	0.2318	0.268	0.245
185	C6H12	3-METHYL-1-PENTENE	84.161	120.20	327.33	495.00	32.90	343.3	0.2452	0.274	0.264
186	C6H12	3-METHYL-cis-2-PENTENE	84.161	138.31	340.85	515.00	32.90	343.0	0.2454	0.264	0.259
187	C6H12	4-METHYL-1-PENTENE	84.161	119.51	327.01	496.00	32.20	345.0	0.2439	0.269	0.239
188	C6H12	4-METHYL-cis-2-PENTENE	84.161	138.30	329.53	499.00	32.20	346.0	0.2432	0.269	0.244
189	C6H12	4-METHYL-trans-2-PENTENE	84.161	132.35	331.75	501.00	32.20	346.0	0.2432	0.267	0.255
190	C6H12N2	TRIETHYLENEDIAMINE	112.175	434.25	447.15	655.00	39.10	382.0	0.2937	0.274	0.460
191	C6H12O	BUTYL VINYL ETHER	100.161	181.25	366.97	536.00	31.20	364.0	0.2752	0.255	0.380
192	C6H12O	CYCLOHEXANOL	100.161	296.60	434.00	625.15	37.49	322.0	0.3111	0.232	0.514
193	C6H12O	1-HEXANAL	100.161	217.15	401.45	579.00	31.10	369.0	0.2714	0.238	0.439
194	C6H12O	ETHYL ISOPROPYL KETONE	100.161	---	386.55	567.00	33.20	369.0	0.2714	0.260	0.391
195	C6H12O	2-HEXANONE	100.161	217.35	400.85	587.05	33.24	369.0	0.2714	0.251	0.397
196	C6H12O	3-HEXANONE	100.161	217.50	396.65	582.82	33.20	364.0	0.2752	0.249	0.376
197	C6H12O	METHYL ISOBUTYL KETONE	100.161	189.15	389.65	571.40	32.73	369.0	0.2714	0.254	0.389
198	C6H12O2	n-PENTYL FORMATE	116.160	199.65	406.60	576.00	31.25	389.0	0.2986	0.254	0.528
199	C6H12O2	n-BUTYL ACETATE	116.160	199.65	399.15	579.65	31.10	389.0	0.2986	0.251	0.410
200	C6H12O2	sec-BUTYL ACETATE	116.160	174.15	385.15	561.00	31.70	389.0	0.2986	0.264	0.406
201	C6H12O2	tert-BUTYL ACETATE	116.160	---	369.15	545.00	31.70	389.0	0.2986	0.272	0.343
202	C6H12O2	ETHYL n-BUTYRATE	116.160	175.15	394.65	571.00	30.60	421.0	0.2759	0.271	0.419
203	C6H12O2	ETHYL ISOBUTYRATE	116.160	185.00	383.00	553.15	30.40	410.0	0.2833	0.271	0.426
204	C6H12O2	ISOBUTYL ACETATE	116.160	174.30	389.80	561.00	31.60	389.0	0.2986	0.264	0.454
205	C6H12O2	n-PROPYL PROPIONATE	116.160	197.25	395.65	578.00	31.10	389.0	0.2986	0.252	0.376
206	C6H12O2	CYCLOHEXYL PEROXIDE	116.160	253.15	490.00	685.00	42.10	342.0	0.3396	0.253	0.751
207	C6H12O2	DIACETONE ALCOHOL	116.160	229.15	441.00	606.00	36.00	387.0	0.3002	0.277	0.757
208	C6H12O2	2-ETHYL BUTYRIC ACID	116.160	258.15	466.95	655.00	34.10	389.0	0.2986	0.244	0.633
209	C6H12O2	n-HEXANOIC ACID	116.160	270.15	478.85	667.00	33.50	389.0	0.2986	0.235	0.670
210	C6H12O3	2-ETHOXYETHYL ACETATE	132.159	211.45	429.45	597.00	24.62	409.0	0.3231	0.203	0.534
211	C6H12O3	HYDROXYCAPROIC ACID	132.159	334.00	576.00	758.00	36.40	402.0	0.3288	0.232	1.163
212	C6H12O3	PARALDEHYDE	132.159	285.75	397.25	579.00	35.00	365.0	0.3621	0.265	0.441
213	C6H12O3	sec-BUTYL GLYCOLATE	132.160	---	450.65	---	---	---	---	---	---
214	C6H13N	CYCLOHEXYLAMINE	99.176	255.45	407.65	615.00	42.00	360.0	0.2755	0.296	0.360
215	C6H13N	HEXAMETHYLENEIMINE	99.176	236.15	404.85	615.00	42.70	361.0	0.2747	0.301	0.330
216	C6H14	2-2-DIMETHYLBUTANE	86.177	174.28	322.88	488.78	30.81	358.8	0.2402	0.272	0.234
217	C6H14	2-3-DIMETHYLBUTANE	86.177	145.19	331.13	499.98	31.27	357.8	0.2409	0.269	0.248

NO	FORMULA	NAME	MW g/mol	T _F K	T _B K	T _C K	P _C bar	V _G cm ³ /mol	ρ _C g/cm ³	Z _C	ω
218	C6H14	n-HEXANE	86.177	177.84	341.88	507.43	30.12	369.9	0.2330	0.264	0.305
219	C6H14	2-METHYLPENTANE	86.177	119.55	333.41	497.50	30.10	366.4	0.2352	0.267	0.278
220	C6H14	3-METHYLPENTANE	86.177	110.25	336.42	504.43	31.24	366.4	0.2352	0.273	0.274
221	C6H14N2O2	LYSINE	146.189	483.00	615.00	821.00	35.30	502.0	0.2912	0.260	1.012
222	C6H14O	2-ETHYL-1-BUTANOL	102.177	158.75	419.65	580.00	34.00	380.0	0.2689	0.268	0.714
223	C6H14O	1-HEXANOL	102.177	228.55	430.15	611.35	35.10	381.3	0.2680	0.263	0.580
224	C6H14O	2-HEXANOL	102.177	223.00	413.04	586.20	34.00	380.0	0.2689	0.265	0.566
225	C6H14O	2-METHYL-1-PENTANOL	102.177	---	421.15	582.00	34.00	380.0	0.2689	0.267	0.726
226	C6H14O	4-METHYL-2-PENTANOL	102.177	---	404.85	574.40	34.70	380.0	0.2689	0.276	0.572
227	C6H14O	n-BUTYL ETHYL ETHER	102.177	170.15	365.35	531.00	29.90	382.0	0.2675	0.259	0.390
228	C6H14O	DIISOPROPYL ETHER	102.177	187.65	341.45	500.05	28.78	386.0	0.2647	0.267	0.338
229	C6H14O	DI-n-PROPYL ETHER	102.177	149.95	362.79	530.60	30.28	382.0	0.2675	0.262	0.370
230	C6H14O	METHYL tert-PENTYL ETHER	102.177	---	359.45	534.00	30.40	382.0	0.2675	0.262	0.301
231	C6H14O2	ACETAL	118.176	173.15	376.75	541.00	29.80	402.0	0.2940	0.266	0.432
232	C6H14O2	2-BUTOXYETHANOL	118.176	203.15	444.47	600.00	32.40	400.0	0.2954	0.260	0.817
233	C6H14O2	1-6-HEXANEDIOL	118.176	315.15	516.15	670.00	36.10	398.0	0.2969	0.258	1.268
234	C6H14O2	HEXYLENE GLYCOL	118.176	223.15	470.65	621.00	40.10	398.0	0.2969	0.309	1.197
235	C6H14O2S	DI-n-PROPYL SULFONE	150.242	303.00	543.00	763.00	31.10	463.0	0.3245	0.227	0.582
236	C6H14O3	DIETHYLENE GLYCOL DIMETHYL ETHER	134.175	203.15	432.91	604.00	28.60	422.0	0.3180	0.240	0.575
237	C6H14O3	DIPROPYLENE GLYCOL	134.175	233.00	504.95	654.00	35.80	415.0	0.3233	0.273	1.198
238	C6H14O3	2-(2-ETHOXYETHOXY)ETHANOL	134.175	195.15	475.15	632.00	31.40	420.0	0.3195	0.251	0.901
239	C6H14O3	TRIMETHYLOLPROPANE	134.175	331.15	562.04	709.00	39.10	416.0	0.3225	0.276	1.543
240	C6H14O4	TRIETHYLENE GLYCOL	150.175	265.79	551.00	700.00	33.20	443.0	0.3390	0.253	1.386
241	C6H14O6	SORBITOL	182.174	370.85	777.00	959.00	46.40	483.0	0.3772	0.281	2.199
242	C6H14S	n-HEXYLMERCAPTAN	118.243	192.62	425.81	623.00	30.80	412.0	0.2870	0.245	0.368
243	C6H15Al	TRIETHYL ALUMINUM	114.167	202.65	458.15	720.15	13.58	230.0	0.4964	0.522	---
244	C6H15Al2Cl3	ETHYL ALUMINUM SESQUICHLORIDE	247.506	253.15	482.15	791.00	---	---	---	---	---
245	C6H15N	DIISOPROPYLAMINE	101.192	176.85	357.05	523.10	32.00	418.0	0.2421	0.308	0.388
246	C6H15N	DI-n-PROPYLAMINE	101.192	210.15	382.00	555.80	36.30	418.0	0.2421	0.328	1.465
247	C6H15N	n-HEXYLAMINE	101.192	251.85	404.65	583.00	31.80	418.0	0.2421	0.274	0.467
248	C6H15N	TRIETHYLAMINE	101.192	158.45	361.92	535.15	30.40	390.0	0.2595	0.266	0.316
249	C6H15NO	6-AMINOHEXANOL	117.191	331.00	508.00	681.00	34.40	436.0	0.2688	0.265	0.970
250	C6H15NO2	DIISOPROPANOLAMINE	133.191	318.15	521.90	672.00	36.00	454.0	0.2934	0.293	1.389
251	C6H15NO3	TRIETHANOLAMINE	149.190	294.35	613.00	787.00	24.50	472.0	0.3161	0.177	1.101
252	C6H15N3	N-AMINOETHYL PIPERAZINE	129.205	254.15	493.55	708.00	38.50	407.0	0.3175	0.266	0.555
253	C6H15O4P	TRIETHYL PHOSPHATE	182.156	216.00	484.15	794.00	10.80	1010.0	0.1804	1.650	---
254	C6H16N2	HEXAMETHYLENEDIAMINE	116.207	313.95	475.04	663.00	32.90	475.0	0.2446	0.284	0.650
255	C6H18N3OP	HEXAMETHYL PHOSPHORAMIDE	179.202	280.15	506.15	---	---	---	---	---	---
256	C6H18N4	TRIETHYLENE TETRAMINE	146.236	285.15	539.65	718.00	31.70	482.0	0.3034	0.256	0.974
257	C6H18OSi2	HEXAMETHYLDISILOXANE	162.379	204.93	373.67	518.70	19.14	601.0	0.2702	0.267	0.418
258	C6H18OSi3	HEXAMETHYLCYCLOTRISILOXANE	222.464	337.15	408.26	554.20	16.63	634.0	0.3509	0.229	0.474
259	C6H19NSi2	HEXAMETHYLDISILAZANE	161.395	---	399.15	544.00	19.20	613.0	0.2633	0.260	0.510
260	C7H3ClF3NO24	4-CHLORO-3-NITROBENZOTRIFLUORIDE	225.554	---	495.15	686.00	27.40	490.0	0.4603	0.235	0.607
261	C7H3Cl2F3	2-4-DICHLOROBENZOTRIFLUORIDE	215.001	247.55	450.65	646.00	28.10	443.0	0.4853	0.232	0.434
262	C7H3Cl2NO	3-4-DICHLOROPHENYL ISOCYANATE	188.012	316.15	501.00	733.00	33.30	456.0	0.4123	0.249	0.335
263	C7H4ClF3	p-CHLOROBENZOTRIFLUORIDE	180.557	237.15	412.15	601.00	30.10	399.0	0.4525	0.240	0.373
264	C7H4Cl2O	m-CHLOROBENZYL CHLORIDE	175.014	280.00	498.00	724.00	36.80	406.0	0.4311	0.248	0.454
265	C7H4F3NO2	3-NITROBENZOTRIFLUORIDE	191.110	272.00	475.93	667.00	28.00	441.0	0.4334	0.223	0.536
266	C7H5ClO	BENZOYL CHLORIDE	140.569	272.65	470.15	697.00	40.60	367.0	0.3830	0.257	0.421
267	C7H5ClO2	o-CHLOROBENZOIC ACID	156.568	415.15	560.15	792.00	40.30	383.0	0.4088	0.234	0.664
268	C7H5Cl3	BENZOTRICHLORIDE	195.475	268.40	486.65	737.00	33.40	447.0	0.4373	0.244	0.260
269	C7H5F3	BENZOTRIFLUORIDE	146.112	244.14	375.20	565.00	33.90	356.0	0.4104	0.257	0.282
270	C7H5N	BENZONITRILE	103.123	260.40	464.15	699.35	42.15	339.0	0.3042	0.246	0.352
271	C7H5NO	PHENYL ISOCYANATE	119.123	243.15	438.75	648.00	40.60	341.0	0.3493	0.257	0.438
272	C7H5N3O6	2-4-6-TRINITROTOLUENE	227.133	354.00	573.00	795.00	30.40	480.0	0.4732	0.221	1.977
273	C7H6Cl2	BENZYL DICHLORIDE	161.030	257.00	487.00	731.00	36.50	404.0	0.3986	0.243	0.326
274	C7H6Cl2	2-4-DICHLOROTOLUENE	161.030	259.65	474.25	705.00	35.90	404.0	0.3986	0.247	0.359
275	C7H6N2O4	2-4-DINITROTOLUENE	182.136	343.00	590.00	814.00	34.00	487.0	0.3740	0.245	0.718
276	C7H6N2O4	2-5-DINITROTOLUENE	182.136	325.65	590.00	814.00	34.00	472.0	0.3859	0.237	0.740
277	C7H6N2O4	2-6-DINITROTOLUENE	182.136	339.00	558.00	770.00	36.00	487.0	0.3740	0.242	0.738
278	C7H6N2O4	3-4-DINITROTOLUENE	182.136	332.00	610.00	842.00	34.00	487.0	0.3740	0.237	0.737
279	C7H6N2O4	3-5-DINITROTOLUENE	182.136	365.65	588.00	814.00	34.00	473.0	0.3851	0.238	0.702
280	C7H6O	BENZALDEHYDE	106.124	247.15	451.90	695.00	46.50	324.0	0.3275	0.261	0.305
281	C7H6O2	BENZOIC ACID	122.123	395.52	522.40	751.00	44.70	339.1	0.3600	0.246	0.604
282	C7H6O2	p-HYDROXYBENZALDEHYDE	122.123	390.15	583.15	844.00	49.90	361.0	0.3383	0.257	0.617
283	C7H6O2	SALICYLALDEHYDE	122.123	266.15	469.65	680.00	49.90	342.0	0.3571	0.302	0.626
284	C7H6O3	SALICYLIC ACID	138.123	431.75	529.00	739.00	51.80	364.0	0.3795	0.307	0.832
285	C7H7Br	p-BROMOTOLUENE	171.037	299.95	457.50	699.00	43.70	379.0	0.4513	0.285	0.318
286	C7H7Cl	BENZYL CHLORIDE	126.585	234.15	452.55	686.00	39.10	360.0	0.3516	0.247	0.314
287	C7H7Cl	o-CHLOROTOLUENE	126.585	236.65	432.30	656.00	39.10	354.0	0.3576	0.254	0.304
288	C7H7Cl	p-CHLOROTOLUENE	126.585	280.65	435.65	660.00	39.10	360.0	0.3516	0.257	0.313
289	C7H7NO	FORMANILIDE	121.139	323.15	544.15	787.00	41.10	382.0	0.3171	0.240	0.545
290	C7H7NO2	m-NITROTOLUENE	137.138	289.20	505.00	734.00	38.00	441.0	0.3110	0.275	0.490
291	C7H7NO2	o-NITROTOLUENE	137.138	269.98	495.64	720.00	38.00	441.0	0.3110	0.280	0.482
292	C7H7NO2	p-NITROTOLUENE	137.138	324.75	511.65	736.00	38.00	441.0	0.3110	0.274	0.541
293	C7H7NO3	o-NITROANISOLE	153.138	283.60	546.15	782.00	37.60	422.0	0.3629	0.244	0.561

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
294	C7H8	TOLUENE	92.141	178.18	383.78	591.79	41.09	315.8	0.2918	0.264	0.264
295	C7H8O	ANISOLE	108.140	235.65	426.73	641.65	41.75	337.0	0.3209	0.264	0.369
296	C7H8O	BENZYL ALCOHOL	108.140	257.85	477.85	677.00	45.50	335.0	0.3228	0.271	0.691
297	C7H8O	m-CRESOL	108.140	285.39	475.43	705.85	45.60	312.0	0.3466	0.242	0.449
298	C7H8O	o-CRESOL	108.140	304.19	464.15	697.55	50.06	282.0	0.3835	0.243	0.434
299	C7H8O	p-CRESOL	108.140	307.93	475.13	704.65	51.50	277.0	0.3904	0.244	0.513
300	C7H8O2	GUAIACOL	124.139	304.65	478.15	697.00	47.30	353.0	0.3517	0.288	0.563
301	C7H8O2	p-METHOXYPHENOL	124.139	329.00	516.00	758.00	49.70	342.0	0.3630	0.270	0.541
302	C7H9N	BENZYLAMINE	107.155	227.15	457.65	683.50	43.20	373.0	0.2873	0.284	0.409
303	C7H9N	2-6-DIMETHYLPYRIDINE	107.155	267.00	417.20	623.75	37.80	316.0	0.3391	0.230	0.350
304	C7H9N	N-METHYLANILINE	107.155	216.15	469.02	701.55	51.98	373.0	0.2873	0.332	0.480
305	C7H9N	m-TOLUIDINE	107.155	242.75	476.55	709.15	41.54	373.0	0.2873	0.263	0.413
306	C7H9N	o-TOLUIDINE	107.155	249.47	473.55	694.15	37.49	373.0	0.2873	0.242	0.442
307	C7H9N	p-TOLUIDINE	107.155	316.90	473.40	693.15	40.00	373.0	0.2873	0.259	0.476
308	C7H10	2-NORBORNENE	94.156	319.40	368.65	583.00	39.30	337.0	0.2794	0.273	0.159
309	C7H10N2	TOLUENEDIAMINE	122.170	371.25	557.15	804.00	43.80	376.0	0.3249	0.246	0.576
310	C7H11NO	CYCLOHEXYL ISOCYANATE	125.170	---	442.15	633.00	34.70	408.0	0.3068	0.269	0.530
311	C7H12O2	n-BUTYL ACRYLATE	128.171	208.55	421.00	598.00	26.30	428.0	0.2995	0.226	0.438
312	C7H12O2	ISOBUTYL ACRYLATE	128.171	212.00	405.15	580.00	29.50	428.0	0.2995	0.262	0.457
313	C7H12O2	n-PROPYL METHACRYLATE	128.171	---	414.00	599.00	29.10	428.0	0.2995	0.250	0.401
314	C7H12O4	DIETHYL MALONATE	160.170	224.25	472.05	653.00	27.80	469.0	0.3415	0.240	0.611
315	C7H14	CYCLOHEPTANE	98.188	265.15	391.94	604.30	38.40	359.0	0.2735	0.274	0.243
316	C7H14	1-1-DIMETHYLCYCLOPENTANE	98.188	203.36	361.00	547.00	34.45	360.0	0.2727	0.273	0.272
317	C7H14	cis-1-2-DIMETHYLCYCLOPENTANE	98.188	219.26	372.68	565.15	34.45	370.0	0.2654	0.271	0.266
318	C7H14	trans-1-2-DIMETHYLCYCLOPENTANE	98.188	155.58	365.02	553.15	34.45	360.0	0.2727	0.270	0.270
319	C7H14	cis-1-3-DIMETHYLCYCLOPENTANE	98.188	139.45	363.92	551.00	34.45	360.0	0.2727	0.271	0.274
320	C7H14	trans-1-3-DIMETHYLCYCLOPENTANE	98.188	139.18	364.88	553.00	34.45	360.0	0.2727	0.270	0.270
321	C7H14	ETHYLCYCLOPENTANE	98.188	134.71	376.62	569.52	33.98	374.5	0.2622	0.269	0.272
322	C7H14	2-ETHYL-1-PENTENE	98.188	168.00	367.15	543.00	29.50	398.0	0.2467	0.260	0.309
323	C7H14	3-ETHYL-1-PENTENE	98.188	145.67	357.26	530.00	30.30	398.0	0.2467	0.274	0.302
324	C7H14	1-HEPTENE	98.188	154.27	366.79	537.29	28.30	413.0	0.2377	0.262	0.331
325	C7H14	cis-2-HEPTENE	98.188	164.00	371.56	549.00	28.40	424.0	0.2316	0.264	0.294
326	C7H14	trans-2-HEPTENE	98.188	163.67	371.10	543.00	28.50	406.0	0.2418	0.256	0.337
327	C7H14	cis-3-HEPTENE	98.188	136.51	368.90	545.00	28.40	421.0	0.2332	0.264	0.295
328	C7H14	trans-3-HEPTENE	98.188	136.52	368.82	540.00	28.50	406.0	0.2418	0.258	0.334
329	C7H14	METHYLCYCLOHEXANE	98.188	146.58	374.08	572.19	34.71	368.0	0.2668	0.269	0.235
330	C7H14	2-METHYL-1-HEXENE	98.188	170.28	364.99	538.00	28.70	398.0	0.2467	0.255	0.309
331	C7H14	3-METHYL-1-HEXENE	98.188	145.00	357.05	528.00	29.50	398.0	0.2467	0.267	0.306
332	C7H14	4-METHYL-1-HEXENE	98.188	131.70	359.88	534.00	30.40	398.0	0.2467	0.273	0.302
333	C7H14	2-3-3-TRIMETHYL-1-BUTENE	98.188	163.30	351.04	531.00	31.40	381.0	0.2577	0.270	0.241
334	C7H14O	DIISOPROPYL KETONE	114.188	204.81	397.55	576.00	30.20	416.0	0.2745	0.262	0.405
335	C7H14O	2-HEPTANONE	114.188	238.15	424.05	611.55	29.20	421.0	0.2712	0.242	0.413
336	C7H14O	1-HEPTANAL	114.188	230.15	425.95	603.00	28.00	421.0	0.2712	0.235	0.487
337	C7H14O	1-METHYLCYCLOHEXANOL	114.188	299.15	430.15	603.00	37.90	414.0	0.2758	0.313	0.683
338	C7H14O	cis-2-METHYLCYCLOHEXANOL	114.188	280.15	438.15	614.00	37.90	414.0	0.2758	0.307	0.679
339	C7H14O	trans-2-METHYLCYCLOHEXANOL	114.188	269.15	439.65	616.00	37.90	414.0	0.2758	0.306	0.683
340	C7H14O	cis-3-METHYLCYCLOHEXANOL	114.188	267.65	441.15	618.00	37.90	414.0	0.2758	0.305	0.704
341	C7H14O	trans-3-METHYLCYCLOHEXANOL	114.188	272.65	441.15	617.00	37.90	414.0	0.2758	0.306	0.697
342	C7H14O	cis-4-METHYLCYCLOHEXANOL	114.188	---	444.15	622.00	37.90	414.0	0.2758	0.303	0.658
343	C7H14O	trans-4-METHYLCYCLOHEXANOL	114.188	---	444.15	622.00	37.90	414.0	0.2758	0.303	0.691
344	C7H14O	5-METHYL-2-HEXANONE	114.188	199.25	417.95	601.00	29.70	421.0	0.2712	0.250	0.434
345	C7H14O2	n-BUTYL PROPIONATE	130.187	183.63	419.75	594.00	28.00	442.0	0.2945	0.251	0.475
346	C7H14O2	ETHYL ISOVALERATE	130.187	173.85	407.45	587.95	28.40	442.0	0.2945	0.257	0.407
347	C7H14O2	ISOPENTYL ACETATE	130.187	194.65	415.25	599.00	28.40	442.0	0.2945	0.252	0.414
348	C7H14O2	n-PENTYL ACETATE	130.187	202.35	422.15	598.00	28.00	442.0	0.2945	0.249	0.490
349	C7H14O2	n-PROPYL n-BUTYRATE	130.187	177.95	416.45	594.00	28.00	442.0	0.2945	0.251	0.448
350	C7H14O2	n-HEPTANOIC ACID	130.187	265.83	496.15	680.00	29.90	442.0	0.2945	0.234	0.717
351	C7H14O3	ETHYL-3-ETHOXYPROPIONATE	146.186	---	438.15	609.00	27.20	462.0	0.3164	0.248	0.578
352	C7H15Br	1-BROMOHEPTANE	179.100	217.05	452.05	651.00	30.80	447.0	0.4007	0.271	0.444
353	C7H15N	N-METHYLCYCLOHEXYLAMINE	113.203	264.65	422.00	622.00	34.90	393.0	0.2880	0.265	0.386
354	C7H16	2-2-DIMETHYLPENTANE	100.204	149.34	352.34	520.50	37.73	416.0	0.2409	0.267	0.288
355	C7H16	2-3-DIMETHYLPENTANE	100.204	---	362.93	537.35	29.08	393.0	0.2550	0.256	0.292
356	C7H16	2-4-DIMETHYLPENTANE	100.204	153.91	353.64	519.79	27.37	418.0	0.2397	0.265	0.302
357	C7H16	3-3-DIMETHYLPENTANE	100.204	138.70	359.21	536.40	29.46	414.0	0.2420	0.273	0.267
358	C7H16	3-ETHYLPENTANE	100.204	154.55	366.62	540.64	28.91	416.0	0.2409	0.268	0.309
359	C7H16	n-HEPTANE	100.204	182.57	371.58	540.26	27.36	431.9	0.2320	0.263	0.351
360	C7H16	2-METHYLHEXANE	100.204	154.90	363.20	530.37	27.34	421.0	0.2380	0.261	0.328
361	C7H16	3-METHYLHEXANE	100.204	153.75	365.00	535.25	28.14	404.0	0.2480	0.255	0.322
362	C7H16	2-2-3-TRIMETHYLBUTANE	100.204	248.57	354.03	531.17	29.54	398.0	0.2518	0.266	0.250
363	C7H16O	1-HEPTANOL	116.203	239.15	449.45	631.90	31.50	435.2	0.2670	0.261	0.587
364	C7H16O	2-HEPTANOL	116.203	243.00	432.35	588.00	30.30	432.0	0.2690	0.268	0.763
365	C7H16O	5-METHYL-1-HEXANOL	116.203	---	445.15	605.00	30.30	432.0	0.2690	0.260	0.781
366	C7H16S	n-HEPTYL MERCAPTAN	132.270	229.92	450.09	645.00	27.70	456.0	0.2901	0.240	0.419
367	C7H17N	1-AMINOHEPTANE	115.219	254.15	430.05	607.00	28.50	471.0	0.2446	0.266	0.511

Appendix E

GAS HEAT CAPACITY FOR C₅ TO C₇ 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	C5Cl6	HEXACHLOROCYCLOPENTADIENE	38.750	8.0546E-01	-1.5519E-03	1.4183E-06	-4.8251E-10	298	1000
2	C5H4O2	FURFURAL	15.470	2.9835E-01	-1.9177E-05	-1.4621E-07	5.9506E-11	100	1500
3	C5H5N	PYRIDINE	23.262	1.1251E-01	3.7351E-04	-4.5402E-07	1.4286E-10	50	1500
4	C5H6	CYCLOPENTADIENE	-25.616	4.2049E-01	-2.7180E-04	7.2995E-08	-3.9537E-12	200	1500
5	C5H6	2-METHYL-1-BUTENE-3-YNE	11.399	3.4714E-01	-2.3506E-04	7.6877E-08	-9.4000E-12	298	1500
6	C5H6	1-PENTENE-3-YNE	9.264	3.3995E-01	-2.3573E-04	8.8403E-08	-1.4533E-11	298	1500
7	C5H6	1-PENTENE-4-YNE	11.588	3.4489E-01	-2.5839E-04	1.0999E-07	-2.0576E-11	298	1500
8	C5H6N2	GLUTARONITRILE	18.975	3.9760E-01	-2.4793E-04	6.6492E-08	-6.1305E-12	298	1500
9	C5H6O2	FURFURYL ALCOHOL	-7.696	5.5491E-01	-4.9754E-04	2.3193E-07	-4.4815E-11	298	1500
10	C5H6O3	GLUTARIC ANHYDRIDE	-39.768	6.2221E-01	-3.8554E-04	1.0999E-07	-1.1564E-11	298	1500
11	C5H6O4	CITRACONIC ACID	-44.280	9.7863E-01	-1.3251E-03	9.3278E-07	-2.5668E-10	298	1200
12	C5H6O4	ITACONIC ACID	-29.874	8.3391E-01	-1.0039E-03	6.4524E-07	-1.6726E-10	298	1200
13	C5H7N	N-METHYLPYRROLE	-42.333	5.9879E-01	-5.0928E-04	2.4282E-07	-4.8924E-11	298	1500
14	C5H7NO2	ETHYL CYANOACETATE	-28.861	6.9064E-01	-6.7310E-04	3.4241E-07	-7.0338E-11	298	1500
15	C5H8	CYCLOPENTENE	-4.355	2.5989E-01	1.1735E-04	-2.3049E-07	7.6078E-11	200	1500
16	C5H8	ISOPRENE	-0.007	4.2828E-01	-3.0377E-04	1.1890E-07	-2.0653E-11	200	1500
17	C5H8	3-METHYL-1,2-BUTADIENE	33.913	2.2132E-01	4.9559E-05	-1.2900E-07	4.1214E-11	150	1500
18	C5H8	1,2-PENTADIENE	15.041	3.3233E-01	-1.2798E-04	-1.0733E-08	1.3140E-11	200	1500
19	C5H8	cis-1,3-PENTADIENE	11.441	3.2718E-01	-1.0552E-04	-3.1107E-08	1.8831E-11	200	1500
20	C5H8	trans-1,3-PENTADIENE	10.384	3.4613E-01	-1.4819E-04	3.3729E-09	9.3660E-12	200	1500
21	C5H8	1,4-PENTADIENE	28.759	2.2687E-01	1.0259E-04	-1.9453E-07	6.2357E-11	100	1500
22	C5H8	2,3-PENTADIENE	29.678	2.8033E-01	-7.3692E-05	-3.3295E-08	1.5621E-11	150	1500
23	C5H8	1-PENTYNE	18.298	3.5705E-01	-2.0856E-04	5.4791E-08	-4.3208E-12	200	1500
24	C5H8	3-METHYL-1-BUTYNE	33.392	2.6136E-01	-1.6275E-05	-9.4718E-08	3.6363E-11	200	1500
25	C5H8N4O12	PENTAERYTHRITOL TETRANITRATE	---	---	---	---	---	---	---
26	C5H8O	CYCLOPENTANONE	-29.270	5.0540E-01	-3.4447E-04	1.3119E-07	-2.6198E-11	298	1500
27	C5H8O	METHYL ISOPROPENYL KETONE	-6.032	4.4160E-01	-2.5697E-04	5.3823E-08	2.4497E-12	298	1200
28	C5H8O2	ACETYLACETONE	-6.071	5.0469E-01	-3.9471E-04	2.1259E-07	-6.0544E-11	298	1200
29	C5H8O2	ALLYL ACETATE	-20.793	6.0941E-01	-5.2082E-04	2.3682E-07	-4.6892E-11	298	1500
30	C5H8O2	ETHYL ACRYLATE	-9.599	5.4466E-01	-4.1029E-04	1.6344E-07	-3.1021E-11	298	1500
31	C5H8O2	METHYL METHACRYLATE	-25.526	6.0628E-01	-5.0627E-04	2.2388E-07	-4.2286E-11	298	1500
32	C5H8O2	VINYL PROPIONATE	-1.977	4.8760E-01	-2.8547E-04	4.8284E-08	7.1078E-12	298	1500
33	C5H8O3	2-HYDROXYETHYL ACRYLATE	-36.842	8.7884E-01	-1.0766E-03	6.9101E-07	-1.7137E-10	298	1200
34	C5H8O3	LEVULINIC ACID	32.518	4.3890E-01	-2.5355E-04	6.9217E-08	-1.1605E-11	298	1500
35	C5H8O3	METHYL ACETOACETATE	-27.476	6.8761E-01	-6.6106E-04	3.5816E-07	-8.1625E-11	298	1500
36	C5H8O4	GLUTARIC ACID	2.795	7.1090E-01	-7.9710E-04	5.4496E-07	-1.6341E-10	298	1200
37	C5H9N	VALERONITRILE	20.430	3.9187E-01	-1.7706E-04	1.0768E-08	9.2411E-12	200	1500
38	C5H9NO	n-BUTYL ISOCYANATE	25.162	3.1973E-01	3.5100E-05	-1.7032E-07	5.8493E-11	298	1100
39	C5H9NO	N-METHYL-2-PYRROLIDONE	-46.964	5.6527E-01	-1.6330E-04	-1.9993E-07	1.2780E-10	298	1200
40	C5H9NO4	L-GLUTAMIC ACID	14.969	6.8061E-01	-5.5977E-04	2.4091E-07	-4.3844E-11	298	1500
41	C5H10	CYCLOPENTANE	19.735	1.1636E-01	5.1261E-04	-5.6745E-07	1.7045E-10	100	1500
42	C5H10	2-METHYL-1-BUTENE	36.231	2.5093E-01	8.9416E-05	-1.8917E-07	6.2160E-11	200	1500
43	C5H10	2-METHYL-2-BUTENE	39.489	1.9866E-01	1.8422E-04	-2.5432E-07	7.7912E-11	200	1500
44	C5H10	3-METHYL-1-BUTENE	34.280	3.1601E-01	-6.1287E-05	-6.6735E-08	2.8688E-11	200	1500
45	C5H10	1-PENTENE	37.101	2.3664E-01	1.1834E-04	-2.1139E-07	6.8054E-11	200	1500
46	C5H10	cis-2-PENTENE	24.729	2.5447E-01	1.1355E-04	-2.1629E-07	7.0502E-11	200	1500
47	C5H10	trans-2-PENTENE	38.859	2.2159E-01	1.3722E-04	-2.1992E-07	6.9261E-11	200	1500
48	C5H10Cl2	1,5-DICHLOROPENTANE	4.347	5.8619E-01	-4.6054E-04	2.0428E-07	-3.9364E-11	298	1500
49	C5H10O	METHYL ISOPROPYL KETONE	-13.343	4.9441E-01	-2.5117E-04	2.5991E-08	9.7133E-12	298	1500
50	C5H10O	2-PENTANONE	42.356	2.7425E-01	6.3786E-05	-1.6870E-07	5.5342E-11	200	1500
51	C5H10O	DIETHYL KETONE	49.800	2.6897E-01	5.0669E-05	-1.5227E-07	4.9510E-11	200	1500
52	C5H10O	VALERALDEHYDE	26.913	3.5952E-01	-6.7847E-05	-7.0728E-08	2.9503E-11	273	1500
53	C5H10O2	n-BUTYL FORMATE	-23.729	6.8205E-01	-6.0993E-04	3.0105E-07	-6.1033E-11	298	1500
54	C5H10O2	ETHYL PROPIONATE	139.382	-4.8565E-01	2.3071E-03	-2.7597E-06	1.0859E-09	298	1000
55	C5H10O2	ISOBUTYL FORMATE	-26.232	6.8785E-01	-6.0138E-04	2.8357E-07	-5.3862E-11	298	1500
56	C5H10O2	ISOPROPYL ACETATE	-45.829	7.9654E-01	-7.9890E-04	4.3031E-07	-9.2988E-11	298	1500
57	C5H10O2	n-PROPYL ACETATE	21.906	4.2733E-01	-1.3858E-04	-5.4238E-08	3.0118E-11	298	1500
58	C5H10O2	METHYL n-BUTYRATE	-39.235	8.0965E-01	-9.2286E-04	6.0084E-07	-1.6118E-10	298	1200
59	C5H10O2	2-METHYLBUTYRIC ACID	-19.156	6.0607E-01	-4.1921E-04	1.3696E-07	-1.7062E-11	298	1500
60	C5H10O2	ISOVALERIC ACID	-5.803	5.9939E-01	-4.6602E-04	1.9713E-07	-3.6253E-11	298	1500
61	C5H10O2	VALERIC ACID	-12.596	6.5474E-01	-5.8609E-04	2.8904E-07	-5.8646E-11	298	1500
62	C5H10O2	TETRAHYDROFURFURYL ALCOHOL	-21.588	7.0118E-01	-6.2383E-04	3.0249E-07	-6.1395E-11	298	1500

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

NO	FORMULA	NAME	A	B	C	D	E	TMIN	TMAX
63	C5H10O2S	3-METHYL SULFOLANE	2.742	4.4985E-01	1.4128E-04	-4.9419E-07	2.1699E-10	298	1200
64	C5H10O3	DIETHYL CARBONATE	---	---	---	---	---	--	--
65	C5H10O3	ETHYL LACTATE	-30.734	8.0038E-01	-8.1025E-04	4.4743E-07	-9.9928E-11	298	1500
66	C5H11Cl	1-CHLOROPENTANE	22.357	4.1358E-01	-1.2716E-04	-4.7751E-08	2.7004E-11	200	1500
67	C5H11N	N-METHYLPYRROLIDINE	-63.618	6.8971E-01	-4.8249E-04	1.6504E-07	-2.1384E-11	298	1500
68	C5H11N	PIPERIDINE	-53.313	7.5541E-01	-5.6470E-04	1.6625E-07	-1.0457E-11	298	1500
69	C5H11NO	tert-BUTYLFORMAMIDE	-18.333	5.7294E-01	-2.9150E-04	-1.2192E-08	3.9907E-11	298	1200
70	C5H12	ISOPENTANE	-0.881	4.7498E-01	-2.4797E-04	6.7512E-08	-8.5343E-12	200	1500
71	C5H12	NEOPENTANE	-17.917	5.7236E-01	-4.1705E-04	2.1158E-07	-5.1006E-11	200	1500
72	C5H12	n-PENTANE	26.671	3.2324E-01	4.2820E-05	-1.6639E-07	5.6036E-11	200	1500
73	C5H12O	2,2-DIMETHYL-1-PROPANOL	-24.052	6.5427E-01	-4.7894E-04	1.6991E-07	-2.1290E-11	298	1500
74	C5H12O	2-METHYL-1-BUTANOL	-19.293	6.3101E-01	-4.7958E-04	1.9533E-07	-3.1575E-11	298	1500
75	C5H12O	2-METHYL-2-BUTANOL	-16.955	6.5298E-01	-5.4260E-04	2.6069E-07	-5.4462E-11	298	1200
76	C5H12O	3-METHYL-1-BUTANOL	17.380	3.8036E-01	9.0875E-05	-3.3684E-07	1.4257E-10	298	1200
77	C5H12O	3-METHYL-2-BUTANOL	-14.366	6.2608E-01	-4.8709E-04	2.1430E-07	-4.1705E-11	298	1500
78	C5H12O	1-PENTANOL	9.175	4.7662E-01	-1.9542E-04	-1.3991E-08	2.0685E-11	200	1500
79	C5H12O	2-PENTANOL	-7.077	5.9369E-01	-4.3971E-04	1.8499E-07	-3.5235E-11	298	1400
80	C5H12O	3-PENTANOL	61.233	7.9840E-02	9.0823E-04	-1.2984E-06	5.4866E-10	298	1000
81	C5H12O	METHYL sec-BUTYL ETHER	-0.104	5.5588E-01	-3.6662E-04	1.3167E-07	-2.0764E-11	298	1500
82	C5H12O	METHYL tert-BUTYL ETHER	39.585	2.8849E-01	1.3825E-04	-2.5131E-07	8.0807E-11	200	1500
83	C5H12O	METHYL ISOBUTYL ETHER	-11.287	5.9389E-01	-4.4085E-04	2.0554E-07	-4.9208E-11	298	1200
84	C5H12O	ETHYL PROPYL ETHER	14.457	4.5609E-01	-1.7751E-04	-1.1636E-08	1.6934E-11	298	1500
85	C5H12O2	ETHYLENE GLYCOL MONOPROPYL ETHER	-16.033	6.8258E-01	-5.7788E-04	2.9935E-07	-7.2869E-11	298	1200
86	C5H12O2	NEOPENTYL GLYCOL	-11.513	6.5964E-01	-4.8149E-04	1.8407E-07	-3.1786E-11	298	1500
87	C5H12O2	1,5-PENTANEDIOL	-2.425	6.1055E-01	-4.3769E-04	1.6872E-07	-2.6880E-11	298	1500
88	C5H12O3	2-(2-METHOXYETHOXY)ETHANOL	-22.744	7.9858E-01	-8.1464E-04	5.3038E-07	-1.5753E-10	298	1200
89	C5H12O4	PENTAERYTHRITOL	-4.675	7.5699E-01	-6.1689E-04	2.7195E-07	-5.3121E-11	298	1400
90	C5H12S	n-PENTYL MERCAPTAN	19.604	4.6839E-01	-2.0875E-04	4.3242E-08	-7.5836E-12	273	1500
91	C5H13N	n-PENTYLAMINE	6.603	5.2073E-01	-2.5708E-04	3.9765E-08	3.5264E-12	298	1500
92	C5H13NO2	METHYL DIETHANOLAMINE	-16.817	7.4349E-01	-5.5635E-04	2.1535E-07	-3.4622E-11	298	1500
93	C6Cl6	HEXACHLOROBENZENE	40.828	6.3403E-01	-7.3328E-04	4.0581E-07	-8.6866E-11	200	1500
94	C6F6	HEXAFLUOROBENZENE	56.398	4.1193E-01	-2.7480E-04	8.4094E-08	-7.9692E-12	200	1500
95	C6H3Cl2NO2	1-CHLORO-2,4-DINITROBENZENE	36.588	5.6182E-01	-3.9302E-04	1.0043E-07	-1.2252E-12	200	1500
96	C6H3Cl2NO2	1,2-DICHLORO-4-NITROBENZENE	20.678	5.6182E-01	-3.9302E-04	1.0043E-07	-1.2252E-12	200	1500
97	C6H3Cl3	1,2,4-TRICHLOROBENZENE	2.547	5.6873E-01	-5.5217E-04	2.6984E-07	-5.2816E-11	200	1500
98	C6H3N3O6	1,3,5-TRINITROBENZENE	52.498	5.6182E-01	-3.9302E-04	1.0043E-07	-1.2252E-12	200	1500
99	C6H4Br2	m-DIBROMOBENZENE	23.494	3.7580E-01	-1.7947E-04	-1.2488E-08	2.2028E-11	150	1500
100	C6H4ClNO2	m-CHLORONITROBENZENE	2.238	5.6182E-01	-3.9302E-04	1.0043E-07	-1.2252E-12	200	1500
101	C6H4ClNO2	o-CHLORONITROBENZENE	5.599	5.4506E-01	-3.6483E-04	8.1076E-08	3.5675E-12	200	1500
102	C6H4ClNO2	p-CHLORONITROBENZENE	2.861	5.6351E-01	-3.9804E-04	1.0486E-07	-2.4547E-12	200	1500
103	C6H4Cl2	m-DICHLOROBENZENE	-9.294	5.4269E-01	-4.8322E-04	2.1721E-07	-3.9293E-11	200	1500
104	C6H4Cl2	o-DICHLOROBENZENE	-9.539	5.4073E-01	-4.7821E-04	2.1330E-07	-3.8284E-11	200	1500
105	C6H4Cl2	p-DICHLOROBENZENE	-9.451	5.4233E-01	-4.8126E-04	2.1537E-07	-3.8775E-11	200	1500
106	C6H4N2O4	m-DINITROBENZENE	18.148	5.6182E-01	-3.9302E-04	1.0043E-07	-1.2252E-12	200	1500
107	C6H4N2O4	o-DINITROBENZENE	18.148	5.6182E-01	-3.9302E-04	1.0043E-07	-1.2252E-12	200	1500
108	C6H4N2O4	p-DINITROBENZENE	18.148	5.6182E-01	-3.9302E-04	1.0043E-07	-1.2252E-12	200	1500
109	C6H5Br	BROMOBENZENE	10.965	3.3493E-01	-7.7630E-05	-9.0065E-08	4.1966E-11	200	1500
110	C6H5Cl	MONOCHLOROBENZENE	27.315	2.4405E-01	9.3748E-05	-2.2377E-07	8.0155E-11	200	1500
111	C6H5ClO	m-CHLOROPHENOL	-30.256	6.6657E-01	-6.5807E-04	3.2782E-07	-6.5085E-11	298	1500
112	C6H5ClO	o-CHLOROPHENOL	-30.256	6.6657E-01	-6.5807E-04	3.2782E-07	-6.5085E-11	298	1500
113	C6H5ClO	p-CHLOROPHENOL	-30.256	6.6657E-01	-6.5807E-04	3.2782E-07	-6.5085E-11	298	1500
114	C6H5Cl2N	3,4-DICHLOROANILINE	-12.710	6.9240E-01	-7.0094E-04	3.5781E-07	-7.2645E-11	298	1500
115	C6H5F	FLUOROBENZENE	-7.810	4.1311E-01	-1.9932E-04	-6.0575E-09	2.0763E-11	200	1500
116	C6H5I	IODOBENZENE	5.014	3.8494E-01	-1.7674E-04	-1.4239E-08	2.1809E-11	200	1500
117	C6H5NO2	NITROBENZENE	-16.202	5.6182E-01	-3.9302E-04	1.0043E-07	-1.2252E-12	200	1500
118	C6H6	BENZENE	-31.368	4.7460E-01	-3.1137E-04	8.5237E-08	-5.0524E-12	200	1500
119	C6H6ClN	m-CHLOROANILINE	-24.493	6.6130E-01	-6.1856E-04	2.9376E-07	-5.6020E-11	298	1500
120	C6H6ClN	o-CHLOROANILINE	-24.493	6.6130E-01	-6.1856E-04	2.9376E-07	-5.6020E-11	298	1500
121	C6H6ClN	p-CHLOROANILINE	-24.135	6.5666E-01	-6.0355E-04	2.7595E-07	-4.8992E-11	298	1200
122	C6H6N2	cis-DICYANO-1-BUTENE	6.870	4.1827E-01	-7.9183E-05	-2.1892E-07	1.2143E-10	298	1000
123	C6H6N2	trans-DICYANO-1-BUTENE	-1.571	5.5288E-01	-4.8007E-04	2.1814E-07	-4.0133E-11	298	1500
124	C6H6N2	1,4-DICYANO-2-BUTENE	39.740	2.7876E-01	1.3446E-04	-3.5716E-07	1.5299E-10	298	1000
125	C6H6N2O2	m-NITROANILINE	12.288	5.7313E-01	-4.5651E-04	1.8410E-07	-2.9867E-11	200	1500
126	C6H6N2O2	o-NITROANILINE	12.288	5.7313E-01	-4.5651E-04	1.8410E-07	-2.9867E-11	200	1500
127	C6H6N2O2	p-NITROANILINE	12.288	5.7313E-01	-4.5651E-04	1.8410E-07	-2.9867E-11	200	1500
128	C6H6O	PHENOL	4.408	3.6338E-01	-6.0417E-05	-1.2794E-07	5.5287E-11	100	1500
129	C6H6O2	1,2-BENZENEDIOL	-24.649	6.2268E-01	-5.0070E-04	1.8696E-07	-2.5672E-11	200	1500
130	C6H6O2	1,3-BENZENEDIOL	-28.476	6.8792E-01	-6.7225E-04	3.3593E-07	-6.7411E-11	200	1500
131	C6H6O2	p-HYDROQUINONE	-23.109	6.6077E-01	-6.4518E-04	3.2817E-07	-6.7604E-11	200	1500
132	C6H6O3	1,2,3-BENZENETRIOL	-23.381	7.5537E-01	-7.6515E-04	3.8498E-07	-7.6871E-11	298	1500
133	C6H6S	PHENYL MERCAPTAN	-5.259	4.4764E-01	-2.3973E-04	2.2703E-08	1.2746E-11	200	1500
134	C6H7N	ANILINE	-22.062	5.7313E-01	-4.5651E-04	1.8410E-07	-2.9867E-11	200	1500

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

NO	FORMULA	NAME	A	B	C	D	E	TMIN	TMAX
135	C6H7N	2-METHYLPYRIDINE	-17.819	4.7591E-01	-2.5380E-04	3.3280E-08	8.7218E-12	200	1500
136	C6H7N	3-METHYLPYRIDINE	-16.136	4.6342E-01	-2.2923E-04	1.6537E-08	1.2749E-11	200	1500
137	C6H7N	4-METHYLPYRIDINE	-18.170	4.7450E-01	-2.4996E-04	3.0282E-08	9.4921E-12	200	1500
138	C6H8	1,3-CYCLOHEXADIENE	9.959	2.5557E-01	2.0432E-04	-3.3043E-07	1.0763E-10	100	1500
139	C6H8	METHYLCYCLOPENTADIENE	-59.926	7.1827E-01	-6.8011E-04	3.3399E-07	-6.6324E-11	298	1500
140	C6H8N2	ADIPONITRILE	46.703	2.1098E-01	6.0849E-04	-1.0564E-06	4.7126E-10	298	1000
141	C6H8N2	METHYLGUTARONITRILE	32.077	4.3754E-01	-2.3741E-04	4.6871E-08	4.8993E-13	298	1500
142	C6H8N2	m-PHENYLENEDIAMINE	-35.663	7.5211E-01	-7.0735E-04	3.3963E-07	-6.5853E-11	298	1500
143	C6H8N2	o-PHENYLENEDIAMINE	-35.663	7.5211E-01	-7.0735E-04	3.3963E-07	-6.5853E-11	298	1500
144	C6H8N2	p-PHENYLENEDIAMINE	-35.663	7.5211E-01	-7.0735E-04	3.3963E-07	-6.5853E-11	298	1500
145	C6H8N2	PHENYLHYDRAZINE	-53.505	7.8460E-01	-7.4455E-04	3.6656E-07	-7.3334E-11	298	1500
146	C6H8N2O	BIS(CYANOETHYL)ETHER	30.043	4.8287E-01	-2.4564E-04	1.9368E-08	1.2919E-11	298	1500
147	C6H8O4	DIMETHYL MALEATE	-1.849	7.6196E-01	-7.8473E-04	4.5797E-07	-1.1125E-10	298	1200
148	C6H8O6	ASCORBIC ACID	-7.357	1.0100E+00	-1.1580E-03	6.7650E-07	-1.5220E-10	298	1500
149	C6H8O7	CITRIC ACID	20.051	8.5219E-01	-8.1655E-04	4.0741E-07	-8.3420E-11	298	1500
150	C6H10	CYCLOHEXENE	11.332	2.5648E-01	2.9121E-04	-4.0917E-07	1.2869E-10	100	1500
151	C6H10	2,3-DIMETHYL-1,3-BUTADIENE	-14.346	6.3345E-01	-5.7820E-04	2.9473E-07	-6.2408E-11	298	1500
152	C6H10	1,5-HEXADIENE	-19.919	5.8801E-01	-4.6457E-04	2.0423E-07	-3.8563E-11	298	1500
153	C6H10	cis,trans-2,4-HEXADIENE	-21.887	5.8531E-01	-4.4663E-04	1.8361E-07	-3.2586E-11	298	1500
154	C6H10	trans,trans-2,4-HEXADIENE	-13.866	5.8123E-01	-4.6720E-04	2.1027E-07	-4.0509E-11	298	1500
155	C6H10	1-HEXYNE	19.611	4.4045E-01	-2.3708E-04	4.1265E-08	3.5316E-12	200	1500
156	C6H10	2-HEXYNE	-3.658	5.1409E-01	-3.7142E-04	1.5649E-07	-2.7818E-11	298	1500
157	C6H10	3-HEXYNE	-12.209	5.5220E-01	-4.4735E-04	2.2254E-07	-4.7781E-11	298	1500
158	C6H10O	CYCLOHEXANONE	-12.337	4.0837E-01	1.0597E-04	-2.9616E-07	1.0088E-10	200	1500
159	C6H10O	MESITYL OXIDE	16.062	5.8779E-01	-6.0312E-04	4.4456E-07	-1.4943E-10	298	1000
160	C6H10O2	epsilon-CAPROLACTONE	-59.878	7.3431E-01	-4.4185E-04	9.0409E-08	3.2030E-12	298	1500
161	C6H10O2	ETHYL METHACRYLATE	-38.063	7.5789E-01	-6.5982E-04	3.0689E-07	-5.9646E-11	298	1500
162	C6H10O2	n-PROPYL ACRYLATE	-34.027	8.8100E-01	-9.6426E-04	5.6512E-07	-1.2909E-10	298	1500
163	C6H10O3	ETHYLACETOACETATE	-38.431	8.1942E-01	-7.5317E-04	3.7707E-07	-7.8132E-11	298	1500
164	C6H10O3	PROPIONIC ANHYDRIDE	29.000	3.6844E-01	3.0361E-04	-6.2082E-07	2.4092E-10	298	1200
165	C6H10O4	ADIPIC ACID	7.418	6.7710E-01	-4.6904E-04	1.4619E-07	-1.5583E-11	298	1500
166	C6H10O4	DIETHYL OXALATE	-63.195	1.0643E+00	-1.1909E-03	6.9357E-07	-1.5592E-10	298	1500
167	C6H10O4	ETHYLENE GLYCOL DIACETATE	-63.207	1.0644E+00	-1.1911E-03	6.9374E-07	-1.5597E-10	298	1500
168	C6H10O4	ETHYLIDENE DIACETATE	-11.375	5.4896E-01	3.3144E-04	-1.0756E-06	5.5152E-10	298	1000
169	C6H11N	HEXANENITRILE	23.213	4.6598E-01	-1.9041E-04	-8.6856E-09	1.7539E-11	200	1500
170	C6H11NO	epsilon-CAPROLACTAM	-10.914	2.7864E-01	6.5610E-04	-9.5916E-07	3.6689E-10	298	1000
171	C6H11NO	CYCLOHEXANONE OXIME	-38.514	6.5385E-01	-2.3559E-04	7.2552E-08	4.5887E-11	298	1500
172	C6H12	CYCLOHEXANE	13.783	2.0742E-01	5.3682E-04	-6.3012E-07	1.8988E-10	100	1500
173	C6H12	2,3-DIMETHYL-1-BUTENE	32.307	4.2869E-01	-1.5601E-04	-2.1440E-08	1.8781E-11	200	1500
174	C6H12	2,3-DIMETHYL-2-BUTENE	50.138	1.9488E-01	3.1558E-04	-3.7082E-07	1.0920E-10	200	1500
175	C6H12	3,3-DIMETHYL-1-BUTENE	37.579	2.8542E-01	1.8034E-04	-3.0375E-07	9.8601E-11	200	1500
176	C6H12	2-ETHYL-1-BUTENE	26.884	3.9566E-01	-5.3867E-05	-1.1252E-07	4.5467E-11	200	1500
177	C6H12	1-HEXENE	32.517	3.5231E-01	2.2971E-05	-1.6592E-07	5.8510E-11	200	1500
178	C6H12	cis-2-HEXENE	35.642	2.9178E-01	1.5778E-04	-2.7413E-07	8.8092E-11	200	1500
179	C6H12	trans-2-HEXENE	49.211	2.6046E-01	1.8185E-04	-2.8038E-07	8.7781E-11	200	1500
180	C6H12	cis-3-HEXENE	58.647	1.3967E-01	4.7553E-04	-5.3528E-07	1.6155E-10	150	1500
181	C6H12	trans-3-HEXENE	66.499	1.6110E-01	3.8543E-04	-4.4785E-07	1.3530E-10	150	1500
182	C6H12	METHYLCYCLOPENTANE	-9.939	4.2528E-01	1.2521E-05	-1.8864E-07	6.4751E-11	200	1500
183	C6H12	2-METHYL-1-PENTENE	35.161	3.5515E-01	1.6698E-05	-1.6387E-07	5.7999E-11	200	1500
184	C6H12	2-METHYL-2-PENTENE	27.059	3.4858E-01	4.7035E-05	-1.9000E-07	6.5743E-11	200	1500
185	C6H12	3-METHYL-1-PENTENE	59.573	2.5875E-01	1.8945E-04	-3.0001E-07	9.6074E-11	150	1500
186	C6H12	3-METHYL-cis-2-PENTENE	58.069	1.6574E-01	4.0178E-04	-4.6769E-07	1.4145E-10	150	1500
187	C6H12	4-METHYL-1-PENTENE	26.362	3.5120E-01	3.9961E-05	-1.8537E-07	6.4392E-11	200	1500
188	C6H12	4-METHYL-cis-2-PENTENE	52.969	2.5164E-01	2.0116E-04	-3.0068E-07	9.5720E-11	200	1500
189	C6H12	4-METHYL-trans-2-PENTENE	39.751	3.7243E-01	-5.1165E-05	-9.8996E-08	3.8818E-11	200	1500
190	C6H12N2	TRIETHYLENEDIAMINE	-124.418	1.0337E+00	-8.2395E-04	3.2203E-07	-4.8974E-11	298	1500
191	C6H12O	BUTYL VINYL ETHER	-1.119	5.8419E-01	-3.7075E-04	1.2882E-07	-2.3385E-11	298	1500
192	C6H12O	CYCLOHEXANOL	17.124	3.3700E-01	2.8176E-04	-4.2713E-07	1.3215E-10	200	1500
193	C6H12O	1-HEXANAL	71.773	2.0294E-01	3.4761E-04	-4.1609E-07	1.2259E-10	200	1500
194	C6H12O	ETHYL ISOPROPYL KETONE	36.515	3.4267E-01	1.4830E-04	-3.4209E-07	1.3148E-10	298	1200
195	C6H12O	2-HEXANONE	45.050	3.5513E-01	4.8896E-05	-1.9813E-07	6.4005E-11	200	1500
196	C6H12O	3-HEXANONE	73.031	2.2148E-01	2.7912E-04	-3.6876E-07	1.1286E-10	150	1500
197	C6H12O	METHYL ISOBUTYL KETONE	2.404	5.8495E-01	-3.7647E-04	1.2418E-07	-1.7051E-11	298	1500
198	C6H12O2	n-PENTYL FORMATE	-30.624	8.1555E-01	-7.4226E-04	3.7578E-07	-7.8511E-11	298	1500
199	C6H12O2	n-BUTYL ACETATE	85.139	7.1561E-02	8.7842E-04	-1.0725E-06	3.7362E-10	298	1200
200	C6H12O2	sec-BUTYL ACETATE	-37.391	8.3030E-01	-6.9627E-04	2.6603E-07	-2.1215E-11	298	1000
201	C6H12O2	tert-BUTYL ACETATE	-66.418	1.0291E+00	-1.1512E-03	7.0828E-07	-1.7774E-10	298	1200
202	C6H12O2	ETHYL n-BUTYRATE	-16.529	7.2624E-01	-5.1890E-04	1.2305E-07	2.3936E-11	298	1200
203	C6H12O2	ETHYL ISOBUTYRATE	-62.802	9.3400E-01	-9.1286E-04	4.8405E-07	-1.0440E-10	298	1500
204	C6H12O2	ISOBUTYL ACETATE	-24.628	7.5868E-01	-5.9783E-04	2.3506E-07	-3.4297E-11	298	1500
205	C6H12O2	n-PROPYL PROPIONATE	-26.162	7.8326E-01	-6.3633E-04	2.2535E-07	-8.0808E-12	298	1200
206	C6H12O2	CYCLOHEXYL PEROXIDE	-66.681	9.6297E-01	-1.0232E-03	7.4423E-07	-2.5645E-10	298	1000

			$C_p = A + B T + C T^2 + D T^3 + E T^4$					$(C_p - \text{joule/g-mol K, } T - K)$	
NO	FORMULA	NAME	A	B	C	D	E	TMIN	TMAX
207	C6H12O2	DIACETONE ALCOHOL	13.030	5.9591E-01	-3.8411E-04	1.5153E-07	-3.8398E-11	298	1200
208	C6H12O2	2-ETHYL BUTYRIC ACID	-44.341	8.5885E-01	-8.2522E-04	4.6805E-07	-1.1743E-10	298	1200
209	C6H12O2	n-HEXANOIC ACID	-9.559	7.4029E-01	-6.6784E-04	3.7713E-07	-1.0030E-10	298	1200
210	C6H12O3	2-ETHOXYETHYL ACETATE	-34.381	8.6550E-01	-7.7015E-04	3.7720E-07	-8.0618E-11	298	1500
211	C6H12O3	HYDROXYCAPROIC ACID	-2.103	7.3513E-01	-5.5705E-04	2.2007E-07	-3.6780E-11	298	1500
212	C6H12O3	PARALDEHYDE	-129.363	1.2890E+00	-1.4032E-03	7.4424E-07	-1.4315E-10	298	1500
213	C6H12O3	sec-BUTYL GLYCOLATE	---	---	---	---	---	---	---
214	C6H13N	CYCLOHEXYLAMINE	-47.225	7.0490E-01	-3.4142E-04	1.8298E-08	1.9665E-11	298	1500
215	C6H13N	HEXAMETHYLENEIMINE	-81.362	7.9390E-01	-4.5964E-04	9.4512E-08	2.5824E-12	298	1400
216	C6H14	2,2-DIMETHYLBUTANE	-1.477	5.5644E-01	-2.4802E-04	4.1433E-08	2.4035E-13	200	1500
217	C6H14	2,3-DIMETHYLBUTANE	-25.999	6.8344E-01	-4.8517E-04	2.1262E-07	-4.3837E-11	200	1500
218	C6H14	n-HEXANE	25.924	4.1927E-01	-1.2491E-05	-1.5916E-07	5.8784E-11	200	1500
219	C6H14	2-METHYLPENTANE	-7.197	6.0097E-01	-3.4094E-04	9.5210E-08	-1.0297E-11	200	1500
220	C6H14	3-METHYLPENTANE	-7.123	5.8327E-01	-3.0338E-04	6.8016E-08	-3.9778E-12	200	1500
221	C6H14N2O2	LYSINE	3.524	8.1910E-01	-6.3474E-04	2.7688E-07	-5.6094E-11	298	1500
222	C6H14O	2-ETHYL-1-BUTANOL	-25.284	7.6092E-01	-6.1315E-04	2.7815E-07	-5.3099E-11	298	1500
223	C6H14O	1-HEXANOL	10.719	5.5767E-01	-2.1818E-04	-3.2298E-08	2.9769E-11	200	1500
224	C6H14O	2-HEXANOL	-8.756	6.7929E-01	-4.4926E-04	1.4008E-07	-1.1453E-11	298	1200
225	C6H14O	2-METHYL-1-PENTANOL	-18.096	7.1113E-01	-5.2110E-04	2.1617E-07	-4.0923E-11	298	1500
226	C6H14O	4-METHYL-2-PENTANOL	-17.282	7.3333E-01	-5.6666E-04	2.4735E-07	-4.7894E-11	298	1500
227	C6H14O	n-BUTYL ETHYL ETHER	10.663	5.7291E-01	-2.7890E-04	3.8539E-08	6.0989E-12	298	1500
228	C6H14O	DIISOPROPYL ETHER	92.068	1.1054E-01	5.8784E-04	-6.1854E-07	1.7855E-10	100	1500
229	C6H14O	DI-n-PROPYL ETHER	-26.082	7.6707E-01	-6.4734E-04	3.3945E-07	-8.3996E-11	298	1200
230	C6H14O	METHYL tert-PENTYL ETHER	-5.816	6.8044E-01	-4.6708E-04	1.7397E-07	-2.8573E-11	298	1500
231	C6H14O2	ACETAL	31.834	3.4539E-01	5.6817E-04	-1.0268E-06	4.4628E-10	298	1000
232	C6H14O2	2-BUTOXYETHANOL	-22.219	8.1143E-01	-7.1242E-04	3.9347E-07	-1.0334E-10	298	1200
233	C6H14O2	1,6-HEXANEDIOL	-2.789	7.0351E-01	-4.9185E-04	1.8516E-07	-3.0221E-11	298	1500
234	C6H14O2	HEXYLENE GLYCOL	-30.746	8.8908E-01	-8.0455E-04	4.0021E-07	-8.2866E-11	298	1500
235	C6H14O2S	DI-n-PROPYL SULFONE	16.469	6.7237E-01	-3.3664E-04	5.5367E-08	4.0249E-12	298	1500
236	C6H14O3	DIETHYLENE GLYCOL DIMETHYL ETHER	-38.307	9.9161E-01	-1.1006E-03	7.7626E-07	-2.4078E-10	298	1200
237	C6H14O3	DIPROPYLENE GLYCOL	-31.988	9.4839E-01	-8.9835E-04	4.8010E-07	-1.1001E-10	298	1200
238	C6H14O3	2-(2-ETHOXYETHOXY)ETHANOL	-15.223	8.0630E-01	-6.0939E-04	2.4852E-07	-4.4531E-11	298	1500
239	C6H14O3	TRIMETHYLOLPROPANE	-14.530	8.3299E-01	-6.6014E-04	2.7694E-07	-4.8128E-11	298	1500
240	C6H14O4	TRIETHYLENE GLYCOL	2.101	7.8650E-01	-5.6060E-04	2.0905E-07	-3.3896E-11	298	1500
241	C6H14O6	SORBITOL	-6.695	1.0042E+00	-7.9252E-04	2.0507E-07	3.0979E-11	298	1200
242	C6H14S	n-HEXYLMERCAPTAN	56.097	3.5459E-01	1.3831E-04	-2.6776E-07	8.5007E-11	200	1500
243	C6H15Al	TRIETHYL ALUMINUM	---	---	---	---	---	---	---
244	C6H15Al2Cl3	TRIETHYL ALUMINUM SESQUICHLORIDE	123.889	2.1683E-01	6.9390E-04	-8.2388E-07	2.5547E-10	100	1500
245	C6H15N	DIISOPROPYLAMINE	-38.690	8.3934E-01	-6.8079E-04	3.1403E-07	-6.5038E-11	298	1500
246	C6H15N	DI-n-PROPYLAMINE	-35.272	8.1873E-01	-6.6672E-04	3.1414E-07	-6.4824E-11	298	1500
247	C6H15N	n-HEXYLAMINE	62.901	3.0756E-01	2.3918E-04	-3.4644E-07	1.0365E-10	200	1500
248	C6H15N	TRIETHYLAMINE	55.793	3.3337E-01	2.2077E-04	-3.4942E-07	1.0838E-10	200	1500
249	C6H15NO	6-AMINOHEXANOL	10.049	6.6024E-01	-3.7498E-04	9.7671E-08	-1.2128E-11	298	1500
250	C6H15NO2	DIISOPROPANOLAMINE	-32.670	9.6179E-01	-8.5944E-04	4.1808E-07	-8.2801E-11	298	1200
251	C6H15NO3	TRIETHANOLAMINE	37.730	4.9155E-01	3.5952E-04	-8.2287E-07	3.5374E-10	298	1200
252	C6H15N3	N-AMINOETHYL PIPERAZINE	-18.325	7.9527E-01	-4.9153E-04	1.3652E-07	-1.2092E-11	298	1500
253	C6H15O4P	TRIETHYL PHOSPHATE	---	---	---	---	---	---	---
254	C6H16N2	HEXAMETHYLENEDIAMINE	8.511	7.1350E-01	-4.7390E-04	2.1163E-07	-6.1825E-11	298	1200
255	C6H18N3OP	HEXAMETHYL PHOSPHORAMIDE	---	---	---	---	---	---	---
256	C6H18N4	TRIETHYLENE TETRAMINE	-26.003	1.0161E+00	-8.1609E-04	3.6628E-07	-7.0398E-11	298	1500
257	C6H18OSi2	HEXAMETHYLDISILOXANE	96.759	5.3023E-01	-1.0701E-04	-1.0135E-07	4.3962E-11	200	1500
258	C6H18O3Si3	HEXAMETHYLCYCLOTRIISILOXANE	42.372	7.1830E-01	-3.5419E-05	-3.1816E-07	1.2408E-10	100	1500
259	C6H19NSi2	HEXAMETHYLDISILAZANE	-10.219	8.5172E-01	-4.3504E-04	6.1843E-08	9.4823E-12	298	1500
260	C7H3ClF3NO24	4-CHLORO-3-NITROBENZOTRIFLUORIDE	2.462	8.0944E-01	-8.0238E-04	3.9826E-07	-7.8100E-11	298	1600
261	C7H3Cl2F3	2,4-DICHLOROBENZOTRIFLUORIDE	-18.588	8.4436E-01	-8.9784E-04	4.7892E-07	-1.0373E-10	298	1200
262	C7H3Cl2NO	3,4-DICHLOROPHENYL ISOCYANATE	-88.252	1.2181E+00	-1.8543E-03	1.3889E-06	-3.9144E-10	298	1200
263	C7H4ClF3	p-CHLOROBENZOTRIFLUORIDE	-32.088	8.0944E-01	-8.0238E-04	3.9826E-07	-7.8100E-11	298	1600
264	C7H4Cl2O	m-CHLOROBENZOYL CHLORIDE	3.438	5.7712E-01	-4.8258E-04	2.0062E-07	-3.3551E-11	298	1500
265	C7H4F3NO2	3-NITROBENZOTRIFLUORIDE	-16.178	8.0944E-01	-8.0238E-04	3.9826E-07	-7.8100E-11	298	1600
266	C7H5ClO	BENZOYL CHLORIDE	-8.923	5.4527E-01	-4.0749E-04	1.4722E-07	-2.0723E-11	298	1500
267	C7H5ClO2	o-CHLOROBENZOIC ACID	8.444	3.3784E-01	3.0050E-04	-6.8672E-07	3.0928E-10	298	1000
268	C7H5Cl3	BENZOTRICHLORIDE	-17.223	7.3674E-01	-7.4806E-04	4.2367E-07	-1.0609E-10	298	1200
269	C7H5F3	BENZOTRIFLUORIDE	-5.571	5.6388E-01	-3.3437E-04	5.2123E-08	1.1313E-11	200	1500
270	C7H5N	BENZONITRILE	-2.624	4.5843E-01	-2.6757E-04	4.3711E-08	7.3182E-12	200	1500
271	C7H5NO	PHENYL ISOCYANATE	-28.586	5.8118E-01	-4.2739E-04	1.4817E-07	-1.9292E-11	298	1500
272	C7H5N3O6	2,4,6-TRINITROTOLUENE	78.953	5.2187E-01	-2.9827E-04	6.1220E-08	1.2576E-12	200	1500
273	C7H6Cl2	BENZYL DICHLORIDE	-23.635	6.5729E-01	-5.5210E-04	2.3709E-07	-4.1699E-11	298	1500
274	C7H6Cl2	2,4-DICHLOROTOLUENE	37.983	2.1821E-01	7.2356E-04	-1.2976E-06	6.0155E-10	298	1000
275	C7H6N2O4	2,4-DINITROTOLUENE	44.603	5.2187E-01	-2.9827E-04	6.1220E-08	1.2576E-12	200	1500
276	C7H6N2O4	2,5-DINITROTOLUENE	44.603	5.2187E-01	-2.9827E-04	6.1220E-08	1.2576E-12	200	1500
277	C7H6N2O4	2,6-DINITROTOLUENE	44.603	5.2187E-01	-2.9827E-04	6.1220E-08	1.2576E-12	200	1500
278	C7H6N2O4	3,4-DINITROTOLUENE	44.603	5.2187E-01	-2.9827E-04	6.1220E-08	1.2576E-12	200	1500

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

NO	FORMULA	NAME	A	B	C	D	E	TMIN	TMAX
279	C7H6N2O4	3,5-DINITROTOLUENE	44.603	5.2187E-01	-2.9827E-04	6.1220E-08	1.2576E-12	200	1500
280	C7H6O	BENZALDEHYDE	-0.890	4.4758E-01	-1.8566E-04	-3.6205E-08	3.1110E-11	200	1500
281	C7H6O2	BENZOIC ACID	16.158	2.8234E-01	1.7811E-04	-3.2176E-07	1.0752E-10	200	1500
282	C7H6O2	p-HYDROXYBENZALDEHYDE	-17.327	6.1293E-01	-3.6141E-04	4.2615E-08	1.8399E-11	298	1200
283	C7H6O2	SALICYLALDEHYDE	-33.117	7.0148E-01	-5.4741E-04	2.0112E-07	-2.8014E-11	298	1500
284	C7H6O3	SALICYLIC ACID	-4.230	4.2572E-01	1.4885E-04	-5.4965E-07	2.6161E-10	298	1000
285	C7H7Br	p-BROMOTOLUENE	-11.148	5.5111E-01	-3.6702E-04	1.0465E-07	-8.5052E-12	298	1500
286	C7H7Cl	BENZYL CHLORIDE	-20.027	5.0561E-01	-3.9247E-04	1.4825E-07	-2.1517E-11	200	1500
287	C7H7Cl	o-CHLOROTOLUENE	-19.597	5.4660E-01	-2.2561E-04	-1.3546E-07	1.0757E-10	298	1000
288	C7H7Cl	p-CHLOROTOLUENE	-19.597	5.4660E-01	-2.2561E-04	-1.3546E-07	1.0757E-10	298	1000
289	C7H7NO	FORMANILIDE	-58.019	7.4752E-01	-6.4061E-04	2.6844E-07	-4.4253E-11	298	1500
290	C7H7NO2	m-NITROTOLUENE	10.253	5.2187E-01	-2.9827E-04	6.1220E-08	1.2576E-12	200	1500
291	C7H7NO2	o-NITROTOLUENE	10.253	5.2187E-01	-2.9827E-04	6.1220E-08	1.2576E-12	200	1500
292	C7H7NO2	p-NITROTOLUENE	10.253	5.2187E-01	-2.9827E-04	6.1220E-08	1.2576E-12	200	1500
293	C7H7NO3	o-NITROANISOLE	-11.742	6.4927E-01	-4.3634E-04	1.1823E-07	-3.1868E-12	298	1200
294	C7H8	TOLUENE	-24.097	5.2187E-01	-2.9827E-04	6.1220E-08	1.2576E-12	200	1500
295	C7H8O	ANISOLE	-46.092	6.4927E-01	-4.3634E-04	1.1823E-07	-3.1868E-12	298	1200
296	C7H8O	BENZYL ALCOHOL	-38.244	5.7295E-01	-1.9618E-04	-1.7885E-07	1.2218E-10	298	1000
297	C7H8O	m-CRESOL	-28.118	6.6639E-01	-5.5684E-04	2.4989E-07	-4.7599E-11	200	1500
298	C7H8O	o-CRESOL	-10.489	5.7475E-01	-3.8585E-04	1.1736E-07	-1.1385E-11	200	1500
299	C7H8O	p-CRESOL	-21.163	6.2005E-01	-4.6259E-04	1.7288E-07	-2.5755E-11	200	1500
300	C7H8O2	GUAIACOL	-53.237	8.0557E-01	-7.1471E-04	3.1975E-07	-5.4471E-11	298	1200
301	C7H8O2	p-METHOXYPHENOL	-55.124	8.2278E-01	-7.6384E-04	3.7503E-07	-7.5815E-11	298	1500
302	C7H9N	BENZYLAMINE	-44.632	7.3792E-01	-6.4144E-04	3.0305E-07	-6.0296E-11	298	1500
303	C7H9N	2,6-DIMETHYLPYRIDINE	-12.959	5.3389E-01	-2.5211E-04	1.2256E-08	1.5481E-11	200	1500
304	C7H9N	N-METHYLANILINE	-63.167	8.2599E-01	-7.5180E-04	3.5552E-07	-6.8719E-11	298	1500
305	C7H9N	m-TOLUIDINE	-15.216	5.9535E-01	-3.8755E-04	1.1831E-07	-1.2703E-11	200	1500
306	C7H9N	o-TOLUIDINE	-15.391	6.2396E-01	-4.3867E-04	1.5449E-07	-2.1698E-11	200	1500
307	C7H9N	p-TOLUIDINE	-18.360	6.1016E-01	-4.1260E-04	1.3537E-07	-1.6747E-11	200	1500
308	C7H10	2-NORBORNENE	-75.556	7.5963E-01	-5.2049E-04	1.6449E-07	-1.7953E-11	298	1500
309	C7H10N2	TOLUENEDIAMINE	-75.447	1.0663E+00	-1.1548E-03	6.1040E-07	-1.1054E-10	298	1500
310	C7H11NO	CYCLOHEXYL ISOCYANATE	-20.869	5.1917E-01	4.6475E-05	-2.9175E-07	1.0386E-10	298	1500
311	C7H12O2	n-BUTYL ACRYLATE	31.423	6.2124E-01	-3.6990E-04	1.0373E-07	-1.7445E-11	298	1000
312	C7H12O2	ISOBUTYL ACRYLATE	-39.964	9.9799E-01	-1.0514E-03	5.9928E-07	-1.3516E-10	298	1500
313	C7H12O2	n-PROPYL METHACRYLATE	-43.005	8.7703E-01	-7.6204E-04	3.5635E-07	-6.9619E-11	298	1500
314	C7H12O4	DIETHYL MALONATE	-85.174	1.2290E+00	-1.3284E-03	7.4897E-07	-1.6575E-10	298	1500
315	C7H14	CYCLOHEPTANE	9.447	3.5261E-01	3.7699E-04	-5.3869E-07	1.6956E-10	100	1500
316	C7H14	1,1-DIMETHYLCYCLOPENTANE	9.329	4.1173E-01	1.8706E-04	-3.7024E-07	1.2310E-10	200	1500
317	C7H14	cis-1,2-DIMETHYLCYCLOPENTANE	10.096	4.1584E-01	1.6872E-04	-3.5294E-07	1.1818E-10	200	1500
318	C7H14	trans-1,2-DIMETHYLCYCLOPENTANE	11.514	4.1203E-01	1.7044E-04	-3.5275E-07	1.1806E-10	200	1500
319	C7H14	cis-1,3-DIMETHYLCYCLOPENTANE	11.486	4.1227E-01	1.6993E-04	-3.5235E-07	1.1795E-10	200	1500
320	C7H14	trans-1,3-DIMETHYLCYCLOPENTANE	11.486	4.1227E-01	1.6993E-04	-3.5235E-07	1.1795E-10	200	1500
321	C7H14	ETHYLCYCLOPENTANE	-28.514	5.7607E-01	-9.4379E-05	-1.6445E-07	6.9435E-11	100	1500
322	C7H14	2-ETHYL-1-PENTENE	7.553	5.5924E-01	-1.9092E-04	-5.9654E-08	3.5819E-11	298	1500
323	C7H14	3-ETHYL-1-PENTENE	2.696	5.6924E-01	-1.9489E-04	-6.2627E-08	3.7450E-11	298	1500
324	C7H14	1-HEPTENE	40.754	3.9922E-01	5.3848E-05	-2.1599E-07	7.4482E-11	200	1500
325	C7H14	cis-2-HEPTENE	-7.099	5.9005E-01	-2.3765E-04	-2.1795E-08	2.4907E-11	200	1500
326	C7H14	trans-2-HEPTENE	22.872	4.6064E-01	-1.9919E-05	-1.7969E-07	6.6169E-11	150	1500
327	C7H14	cis-3-HEPTENE	-25.417	6.7669E-01	-3.7697E-04	7.3028E-08	1.3960E-12	200	1500
328	C7H14	trans-3-HEPTENE	1.557	5.6602E-01	-1.9660E-04	-5.5257E-08	3.4487E-11	150	1500
329	C7H14	METHYLCYCLOHEXANE	4.296	4.2716E-01	2.1058E-04	-3.9987E-07	1.3121E-10	200	1500
330	C7H14	2-METHYL-1-HEXENE	13.419	5.3960E-01	-1.7371E-04	-6.3050E-08	3.5189E-11	298	1500
331	C7H14	3-METHYL-1-HEXENE	2.696	5.6924E-01	-1.9489E-04	-6.2627E-08	3.7450E-11	298	1500
332	C7H14	4-METHYL-1-HEXENE	-21.774	7.0339E-01	-4.4459E-04	1.2769E-07	-1.3424E-11	150	1500
333	C7H14	2,3,3-TRIMETHYL-1-BUTENE	0.695	6.0287E-01	-2.3415E-04	-4.8958E-08	3.6689E-11	298	1500
334	C7H14O	DIISOPROPYL KETONE	-59.457	8.9163E-01	-7.3368E-04	3.3507E-07	-6.4643E-11	298	1500
335	C7H14O	2-HEPTANONE	77.352	2.5365E-01	3.8252E-04	-4.9648E-07	1.4916E-10	150	1500
336	C7H14O	1-HEPTANAL	76.088	2.6868E-01	3.5354E-04	-4.5649E-07	1.3757E-10	200	1500
337	C7H14O	1-METHYLCYCLOHEXANOL	-54.565	8.4577E-01	-5.7323E-04	2.3275E-07	-5.9702E-11	298	1200
338	C7H14O	cis-2-METHYLCYCLOHEXANOL	-47.283	7.6999E-01	-3.7628E-04	3.6819E-08	7.7738E-12	298	1200
339	C7H14O	trans-2-METHYLCYCLOHEXANOL	-47.283	7.6999E-01	-3.7628E-04	3.6819E-08	7.7738E-12	298	1200
340	C7H14O	cis-3-METHYLCYCLOHEXANOL	-47.283	7.6999E-01	-3.7628E-04	3.6819E-08	7.7738E-12	298	1200
341	C7H14O	trans-3-METHYLCYCLOHEXANOL	-47.283	7.6999E-01	-3.7628E-04	3.6819E-08	7.7738E-12	298	1200
342	C7H14O	cis-4-METHYLCYCLOHEXANOL	-47.283	7.6999E-01	-3.7628E-04	3.6819E-08	7.7738E-12	298	1200
343	C7H14O	trans-4-METHYLCYCLOHEXANOL	-47.283	7.6999E-01	-3.7628E-04	3.6819E-08	7.7738E-12	298	1200
344	C7H14O	5-METHYL-2-HEXANONE	-3.763	7.0117E-01	-4.7468E-04	1.8106E-07	-3.3882E-11	298	1200
345	C7H14O2	n-BUTYL PROPIONATE	-3.593	7.7324E-01	-5.9004E-04	2.9563E-07	-8.6992E-11	298	1200
346	C7H14O2	ETHYL ISOVALERATE	-45.699	9.9698E-01	-9.7130E-04	5.3585E-07	-1.2593E-10	298	1200
347	C7H14O2	ISOPENTYL ACETATE	-51.790	9.8897E-01	-9.0976E-04	4.6383E-07	-1.0053E-10	298	1500
348	C7H14O2	n-PENTYL ACETATE	-31.967	8.9188E-01	-7.5408E-04	3.6684E-07	-8.2457E-11	298	1200
349	C7H14O2	n-PROPYL n-BUTYRATE	-8.783	8.0270E-01	-6.4913E-04	3.4629E-07	-1.0270E-10	298	1200
350	C7H14O2	n-HEPTANOIC ACID	11.779	6.9196E-01	-4.1039E-04	1.1266E-07	-1.5295E-11	298	1500

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

NO	FORMULA	NAME	A	B	C	D	E	TMIN	TMAX
351	C7H14O3	ETHYL-3-ETHOXYPROPIONATE	-62.701	1.1653E+00	-1.2886E-03	8.0077E-07	-2.0569E-10	298	1200
352	C7H15Br	1-BROMOHEPTANE	-11.271	7.7970E-01	-5.4848E-04	1.9542E-07	-2.5440E-11	298	1200
353	C7H15N	N-METHYLCYCLOHEXYLAMINE	-59.516	8.3575E-01	-4.3148E-04	4.6928E-08	1.6571E-11	298	1500
354	C7H16	2,2-DIMETHYLPENTANE	-19.277	7.6888E-01	-5.1678E-04	2.0476E-07	-3.7168E-11	200	1500
355	C7H16	2,3-DIMETHYLPENTANE	38.654	3.7259E-01	2.7632E-04	-4.3148E-07	1.3811E-10	100	1500
356	C7H16	2,4-DIMETHYLPENTANE	-32.996	8.7352E-01	-7.3286E-04	3.6633E-07	-7.9787E-11	200	1500
357	C7H16	3,3-DIMETHYLPENTANE	-23.909	7.8329E-01	-5.3992E-04	2.2604E-07	-4.4324E-11	200	1500
358	C7H16	3-ETHYLPENTANE	19.245	5.5072E-01	-1.4055E-04	-8.2482E-08	3.9487E-11	200	1500
359	C7H16	n-HEPTANE	26.984	5.0387E-01	-4.4748E-05	-1.6835E-07	6.5183E-11	200	1500
360	C7H16	2-METHYLHEXANE	-3.249	6.6625E-01	-3.3836E-04	6.0489E-08	2.5385E-12	200	1500
361	C7H16	3-METHYLHEXANE	-12.841	7.1358E-01	-4.2021E-04	1.1997E-07	-1.2906E-11	200	1500
362	C7H16	2,2,3-TRIMETHYLBUTANE	-21.150	7.4663E-01	-4.6699E-04	1.7923E-07	-3.4265E-11	200	1500
363	C7H16O	1-HEPTANOL	11.810	6.4236E-01	-2.4939E-04	-4.3649E-08	3.7035E-11	200	1500
364	C7H16O	2-HEPTANOL	-28.784	8.8407E-01	-7.1442E-04	3.2639E-07	-6.5218E-11	298	1500
365	C7H16O	5-METHYL-1-HEXANOL	0.274	6.8732E-01	-3.1154E-04	-1.1838E-08	3.5683E-11	298	1200
366	C7H16S	n-HEPTYL MERCAPTAN	59.314	4.3814E-01	8.8964E-05	-2.6174E-07	8.7398E-11	200	1500
367	C7H17N	1-AMINOHEPTANE	-1.435	7.4857E-01	-4.4543E-04	1.3200E-07	-1.8684E-11	298	1500

Appendix F

COMPOUND LIST BY FORMULA

CBrClF2	BROMOCHLORODIFLUOROMETHANE.....	1(Vol 1)	C2H2Cl2O	CHLOROACETYL CHLORIDE.....	71(Vol 1)
CBrCl3	BROMOTRICHLOROMETHANE.....	2(Vol 1)	C2H2Cl2O	DICHLOROACETALDEHYDE.....	72(Vol 1)
CBrF3	BROMOTRIFLUOROMETHANE.....	3(Vol 1)	C2H2Cl2O2	DICHLOROACETIC ACID.....	73(Vol 1)
CBr2F2	DIBROMODIFLUOROMETHANE.....	4(Vol 1)	C2H2Cl3F	1,1,1-TRICHLOROFLUOROETHANE.....	74(Vol 1)
CClF3	CHLOROTRIFLUOROMETHANE.....	5(Vol 1)	C2H2Cl4	1,1,1,2-TETRACHLOROETHANE.....	75(Vol 1)
CClN	CYANOGEN CHLORIDE.....	6(Vol 1)	C2H2Cl4	1,1,2,2-TETRACHLOROETHANE.....	76(Vol 1)
CCl2F2	DICHLORODIFLUOROMETHANE.....	7(Vol 1)	C2H2F2	1,1-DIFLUOROETHYLENE.....	77(Vol 1)
CCl2O	PHOSGENE.....	8(Vol 1)	C2H2F4	1,1,1,2-TETRAFLUOROETHANE.....	78(Vol 1)
CCl3F	TRICHLOROFLUOROMETHANE.....	9(Vol 1)	C2H2O	KETENE.....	79(Vol 1)
CCl4	CARBON TETRACHLORIDE.....	10(Vol 1)	C2H2O4	OXALIC ACID.....	80(Vol 1)
CF2O	CARBONYL FLUORIDE.....	11(Vol 1)	C2H3Br	VINYL BROMIDE.....	81(Vol 1)
CF4	CARBON TETRAFLUORIDE.....	12(Vol 1)	C2H3Cl	VINYL CHLORIDE.....	82(Vol 1)
CHBr3	TRIBROMOMETHANE.....	13(Vol 1)	C2H3ClF2	1-CHLORO-1,1-DIFLUOROETHANE.....	83(Vol 1)
CHClF2	CHLORODIFLUOROMETHANE.....	14(Vol 1)	C2H3ClO	ACETYL CHLORIDE.....	84(Vol 1)
CHCl2F	DICHLOROFLUOROMETHANE.....	15(Vol 1)	C2H3ClO	CHLOROACETALDEHYDE.....	85(Vol 1)
CHCl3	CHLOROFORM.....	16(Vol 1)	C2H3ClO2	CHLOROACETIC ACID.....	86(Vol 1)
CHF3	TRIFLUOROMETHANE.....	17(Vol 1)	C2H3ClO2	METHYL CHLOROFORMATE.....	87(Vol 1)
CHN	HYDROGEN CYANIDE.....	18(Vol 1)	C2H3Cl3	1,1,1-TRICHLOROETHANE.....	88(Vol 1)
CH2BrCl	BROMOCHLOROMETHANE.....	19(Vol 1)	C2H3Cl3	1,1,2-TRICHLOROETHANE.....	89(Vol 1)
CH2Br2	DIBROMOMETHANE.....	20(Vol 1)	C2H3F	VINYL FLUORIDE.....	90(Vol 1)
CH2Cl2	DICHLOROMETHANE.....	21(Vol 1)	C2H3F3	1,1,1-TRIFLUOROETHANE.....	91(Vol 1)
CH2F2	DIFLUOROMETHANE.....	22(Vol 1)	C2H3N	ACETONITRILE.....	92(Vol 1)
CH2I2	DIIODOMETHANE.....	23(Vol 1)	C2H3NO	METHYL ISOCYANATE.....	93(Vol 1)
CH2O	FORMALDEHYDE.....	24(Vol 1)	C2H4	ETHYLENE.....	94(Vol 1)
CH2O2	FORMIC ACID.....	25(Vol 1)	C2H4Br2	1,1-DIBROMOETHANE.....	95(Vol 1)
CH3Br	METHYL BROMIDE.....	26(Vol 1)	C2H4Br2	1,2-DIBROMOETHANE.....	96(Vol 1)
CH3Cl	METHYL CHLORIDE.....	27(Vol 1)	C2H4Cl2	1,1-DICHLOROETHANE.....	97(Vol 1)
CH3Cl3Si	METHYL TRICHLOROSILANE.....	28(Vol 1)	C2H4Cl2	1,2-DICHLOROETHANE.....	98(Vol 1)
CH3F	METHYL FLUORIDE.....	29(Vol 1)	C2H4Cl2O	BIS(CHLOROMETHYL)ETHER.....	99(Vol 1)
CH3I	METHYL IODIDE.....	30(Vol 1)	C2H4F2	1,1-DIFLUOROETHANE.....	100(Vol 1)
CH3NO	FORMAMIDE.....	31(Vol 1)	C2H4F2	1,2-DIFLUOROETHANE.....	101(Vol 1)
CH3NO2	NITROMETHANE.....	32(Vol 1)	C2H4O	ACETALDEHYDE.....	102(Vol 1)
CH4	METHANE.....	33(Vol 1)	C2H4O	ETHYLENE OXIDE.....	103(Vol 1)
CH4Cl2Si	METHYL DICHLOROSILANE.....	34(Vol 1)	C2H4O2	ACETIC ACID.....	104(Vol 1)
CH4O	METHANOL.....	35(Vol 1)	C2H4O2	METHYL FORMATE.....	105(Vol 1)
CH4O3S	METHANESULFONIC ACID.....	36(Vol 1)	C2H5Br	BROMOETHANE.....	106(Vol 1)
CH4S	METHYL MERCAPTAN.....	37(Vol 1)	C2H5Cl	ETHYL CHLORIDE.....	107(Vol 1)
CH5ClSi	METHYL CHLOROSILANE.....	38(Vol 1)	C2H5ClO	2-CHLOROETHANOL.....	108(Vol 1)
CH5N	METHYLAMINE.....	39(Vol 1)	C2H5F	ETHYL FLUORIDE.....	109(Vol 1)
CH6Si	METHYL SILANE.....	40(Vol 1)	C2H5I	ETHYL IODIDE.....	110(Vol 1)
CN4O8	TETRANITROMETHANE.....	41(Vol 1)	C2H5N	ETHYLENEIMINE.....	111(Vol 1)
CO	CARBON MONOXIDE.....	42(Vol 1)	C2H5NO	ACETAMIDE.....	112(Vol 1)
COS	CARBONYL SULFIDE.....	43(Vol 1)	C2H5NO	N-METHYLFORMAMIDE.....	113(Vol 1)
CO2	CARBON DIOXIDE.....	44(Vol 1)	C2H5NO2	NITROETHANE.....	114(Vol 1)
CS2	CARBON DISULFIDE.....	45(Vol 1)	C2H6	ETHANE.....	115(Vol 1)
C2BrF3	BROMOTRIFLUOROETHYLENE.....	46(Vol 1)	C2H6AlCl	DIMETHYLALUMINUM CHLORIDE.....	116(Vol 1)
C2Br2F4	1,2-DIBROMOTETRAFLUOROETHANE.....	47(Vol 1)	C2H6O	DIMETHYL ETHER.....	117(Vol 1)
C2ClF3	CHLOROTRIFLUOROETHYLENE.....	48(Vol 1)	C2H6O	ETHANOL.....	118(Vol 1)
C2ClF5	CHLOROPENTAFLUOROETHANE.....	49(Vol 1)	C2H6O2	DIMETHYL SULFOXIDE.....	119(Vol 1)
C2Cl2F4	1,2-DICHLOROTETRAFLUOROETHANE.....	50(Vol 1)	C2H6O2	ETHYLENE GLYCOL.....	120(Vol 1)
C2Cl3F3	1,1,2-TRICHLOROTRIFLUOROETHANE.....	51(Vol 1)	C2H6O4S	DIMETHYL SULFATE.....	121(Vol 1)
C2Cl4	TETRACHLOROETHYLENE.....	52(Vol 1)	C2H6S	DIMETHYL SULFIDE.....	122(Vol 1)
C2Cl4F2	1,1,2,2-TETRACHLORODIFLUOROETHANE.....	53(Vol 1)	C2H6S	ETHYL MERCAPTAN.....	123(Vol 1)
C2Cl4O	TRICHLOROACETYL CHLORIDE.....	54(Vol 1)	C2H6S2	DIMETHYL DISULFIDE.....	124(Vol 1)
C2Cl6	HEXACHLOROETHANE.....	55(Vol 1)	C2H7N	DIMETHYLAMINE.....	125(Vol 1)
C2F4	TETRAFLUOROETHYLENE.....	56(Vol 1)	C2H7N	ETHYLAMINE.....	126(Vol 1)
C2F6	HEXAFLUOROETHANE.....	57(Vol 1)	C2H7NO	MONOETHANOLAMINE.....	127(Vol 1)
C2HBrClF3	HALOTHANE.....	58(Vol 1)	C2H8N2	ETHYLENEDIAMINE.....	128(Vol 1)
C2HClF2	2-CHLORO-1,1-DIFLUOROETHYLENE.....	59(Vol 1)	C2H8Si	DIMETHYL SILANE.....	129(Vol 1)
C2HCl3	TRICHLOROETHYLENE.....	60(Vol 1)	C2N2	CYANOGEN.....	130(Vol 1)
C2HCl3O	DICHLOROACETYL CHLORIDE.....	61(Vol 1)	C3F6	HEXAFLUOROPROPYLENE.....	131(Vol 1)
C2HCl3O	TRICHLOROACETALDEHYDE.....	62(Vol 1)	C3F6O	HEXAFLUOROACETONE.....	132(Vol 1)
C2HCl5	PENTACHLOROETHANE.....	63(Vol 1)	C3F8	OCTAFLUOROPROPANE.....	133(Vol 1)
C2HF3O2	TRIFLUOROACETIC ACID.....	64(Vol 1)	C3H2N2	MALONONITRILE.....	134(Vol 1)
C2HF5	PENTAFLUOROETHANE.....	65(Vol 1)	C3H3Cl	PROPARGYL CHLORIDE.....	135(Vol 1)
C2H2	ACETYLENE.....	66(Vol 1)	C3H3N	ACRYLONITRILE.....	136(Vol 1)
C2H2Br4	1,1,2,2-TETRABROMOETHANE.....	67(Vol 1)	C3H3NO	OXAZOLE.....	137(Vol 1)
C2H2Cl2	1,1-DICHLOROETHYLENE.....	68(Vol 1)	C3H4	METHYLACETYLENE.....	138(Vol 1)
C2H2Cl2	cis-1,2-DICHLOROETHYLENE.....	69(Vol 1)	C3H4	PROPADIENE.....	139(Vol 1)
C2H2Cl2	trans-1,2-DICHLOROETHYLENE.....	70(Vol 1)	C3H4Cl2	2,3-DICHLOROPROPENE.....	140(Vol 1)

C3H4O	ACROLEIN.....	141(Vol 1)	C4H4O3	SUCCINIC ANHYDRIDE.....	219(Vol 1)
C3H4O	PROPARGYL ALCOHOL.....	142(Vol 1)	C4H4O4	FUMARIC ACID.....	220(Vol 1)
C3H4O2	ACRYLIC ACID.....	143(Vol 1)	C4H4S	MALEIC ACID.....	221(Vol 1)
C3H4O2	BETA-PROPIOLACTONE.....	144(Vol 1)	C4H4S	THIOPHENE.....	222(Vol 1)
C3H4O2	VINYL FORMATE.....	145(Vol 1)	C4H5Cl	CHLOROPRENE.....	223(Vol 1)
C3H4O3	ETHYLENE CARBONATE.....	146(Vol 1)	C4H5N	trans-CROTONITRILE.....	224(Vol 1)
C3H4O3	PYRUVIC ACID.....	147(Vol 1)	C4H5N	cis-CROTONITRILE.....	225(Vol 1)
C3H5Cl	2-CHLOROPROPENE.....	148(Vol 1)	C4H5N	METHACRYLONITRILE.....	226(Vol 1)
C3H5Cl	3-CHLOROPROPENE.....	149(Vol 1)	C4H5N	PYRROLE.....	227(Vol 1)
C3H5ClO	alpha-EPICHLOROHYDRIN.....	150(Vol 1)	C4H5N	VINYLAACETONITRILE.....	228(Vol 1)
C3H5ClO2	METHYL CHLOROACETATE.....	151(Vol 1)	C4H5NO2	METHYL CYANOACETATE.....	229(Vol 1)
C3H5ClO2	ETHYL CHLOROFORMATE.....	152(Vol 1)	C4H6	1,2-BUTADIENE.....	230(Vol 1)
C3H5Cl3	1,2,3-TRICHLOROPROPANE.....	153(Vol 1)	C4H6	1,3-BUTADIENE.....	231(Vol 1)
C3H5N	PROPIONITRILE.....	154(Vol 1)	C4H6	DIMETHYLACETYLENE.....	232(Vol 1)
C3H5NO	ACRYLAMIDE.....	155(Vol 1)	C4H6	ETHYLACETYLENE.....	233(Vol 1)
C3H5NO	HYDRACRYLONITRILE.....	156(Vol 1)	C4H6Cl2	1,3-DICHLORO-trans-2-BUTENE.....	234(Vol 1)
C3H5NO	LACTONITRILE.....	157(Vol 1)	C4H6Cl2	1,4-DICHLORO-cis-2-BUTENE.....	235(Vol 1)
C3H5N3O9	NITROGLYCERINE.....	158(Vol 1)	C4H6Cl2	1,4-DICHLORO-trans-2-BUTENE.....	236(Vol 1)
C3H6	CYCLOPROPANE.....	159(Vol 1)	C4H6Cl2	3,4-DICHLORO-1-BUTENE.....	237(Vol 1)
C3H6	PROPYLENE.....	160(Vol 1)	C4H6O	trans-CROTONALDEHYDE.....	238(Vol 1)
C3H6Cl2	1,1-DICHLOROPROPANE.....	161(Vol 1)	C4H6O	2,5-DIHYDROFURAN.....	239(Vol 1)
C3H6Cl2	1,2-DICHLOROPROPANE.....	162(Vol 1)	C4H6O	DIVINYL ETHER.....	240(Vol 1)
C3H6Cl2	1,3-DICHLOROPROPANE.....	163(Vol 2)	C4H6O	METHACROLEIN.....	241(Vol 1)
C3H6O	ACETONE.....	164(Vol 1)	C4H6O2	2-BUTYNE-1,4-DIOL.....	242(Vol 1)
C3H6O	ALLYL ALCOHOL.....	165(Vol 1)	C4H6O2	gamma-BUTYROLACTONE.....	243(Vol 1)
C3H6O	METHYL VINYL ETHER.....	166(Vol 1)	C4H6O2	cis-CROTONIC ACID.....	244(Vol 1)
C3H6O	n-PROPIONALDEHYDE.....	167(Vol 1)	C4H6O2	trans-CROTONIC ACID.....	245(Vol 1)
C3H6O	1,2-PROPYLENE OXIDE.....	168(Vol 1)	C4H6O2	METHACRYLIC ACID.....	246(Vol 1)
C3H6O	1,3-PROPYLENE OXIDE.....	169(Vol 1)	C4H6O2	METHYL ACRYLATE.....	247(Vol 1)
C3H6O2	ETHYL FORMATE.....	170(Vol 1)	C4H6O2	VINYL ACETATE.....	248(Vol 1)
C3H6O2	METHYL ACETATE.....	171(Vol 1)	C4H6O3	ACETIC ANHYDRIDE.....	249(Vol 1)
C3H6O2	PROPIONIC ACID.....	172(Vol 1)	C4H6O4	SUCCINIC ACID.....	250(Vol 1)
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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: 440 C₅H₁₂ n-PENTANE

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	-100.00	0.208	0.022	-242.63	-0.478
500.0	0.00	0.171	0.023	-196.52	-0.365
500.0	100.00	0.152	0.025	-144.08	-0.262
500.0	200.00	0.144	0.028	-84.27	-0.164
500.0	300.00	0.151	0.034	-14.40	-0.065
500.0	400.00	0.476	0.122	113.90	0.091
500.0	500.00	0.724	0.207	193.40	0.179
500.0	1000.00	0.963	0.418	580.50	0.501
3000.0	-100.00	1.232	0.022	-233.98	-0.482
3000.0	0.00	1.008	0.023	-188.53	-0.371
3000.0	100.00	0.875	0.024	-137.40	-0.270
3000.0	200.00	0.797	0.026	-80.30	-0.177
3000.0	300.00	0.758	0.029	-17.09	-0.087
3000.0	400.00	0.751	0.032	52.18	-0.002
3000.0	500.00	0.772	0.037	127.06	0.080
3000.0	1000.00	1.006	0.073	549.91	0.433
10000.0	-100.00	4.024	0.022	-209.14	-0.491
10000.0	0.00	3.244	0.022	-164.63	-0.382
10000.0	100.00	2.757	0.023	-114.95	-0.285
10000.0	200.00	2.431	0.024	-60.03	-0.194
10000.0	300.00	2.204	0.025	0.06	-0.110
10000.0	400.00	2.041	0.026	65.15	-0.029
10000.0	500.00	1.922	0.027	134.97	0.047
10000.0	1000.00	1.649	0.036	544.22	0.388