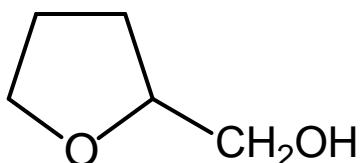




**PENN**  
Specialty Chemicals, Inc.  
Chemicals From Renewable Resources

## TETRAHYDROFURFURYL ALCOHOL



*The Furan Chemistry Specialists*

Environmentally Friendly, Biodegradable Solvent for:  
Biocide and Pesticide Formulations  
Stripping Formulations  
Electronic Cleaner Formulations  
Coatings, Dyes and Printing Ink  
Epoxy Curing Agent

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# TETRAHYDROFURFURYL ALCOHOL

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The information in this bulletin is based on data currently available to us and is thought to be correct.

Penn Specialty Chemicals, Inc. MAKES NO WARRANTIES OF MERCHANTABILITY OR FITNESS FOR A PARTICULAR PURPOSE, OR ANY OTHER EXPRESS OR IMPLIED WARRANTY. BUYER ASSUMES ALL RISK AND LIABILITY RESULTING FROM USE OF PENN SPECIALTY CHEMICALS, INC. PRODUCTS.

MATERIAL SAFETY DATA SHEETS AND OTHER PRODUCT LITERATURE SHOULD ALWAYS BE READ AND UNDERSTOOD PRIOR TO WORKING WITH PENN SPECIALTY CHEMICALS, INC. PRODUCTS.

## **Introduction**

THFA<sup>®</sup> tetrahydrofurfuryl alcohol is an environmentally friendly, naturally derived, biodegradable, water-miscible specialty solvent!

At Penn Specialty Chemicals, we share a growing concern in the chemical industry regarding toxicity and the environment. This concern has revived an interest in the use of “environmentally-friendly” products such as THFA<sup>®</sup>.

Corncocks, oat hulls, and sugar cane bagasse are the raw materials used to manufacture furfural and its derivatives, such as THFA<sup>®</sup>. Through the use of these annually renewable agricultural byproducts, Penn Specialty Chemicals is utilizing replenishable resources!

The advantages of using THFA<sup>®</sup> as a solvent are:

- EPA-approved solvent
- Not “photochemically reactive”
- Readily biodegradable
- Water miscible
- High flash point
- High boiling point
- Low freezing point
- Chemical and thermal stability
- High solvency for organic and inorganic materials

## **Applications**

### **The “Solvent of Choice” for Biocide and Pesticide Formulations**

THFA<sup>®</sup> is the “solvent of choice” for a variety of agricultural applications including pest control, weed control, and growth regulation. THFA<sup>®</sup> outperforms other solvents by providing superior solubility for biologically active materials including phosphates, carbamates, and acetamides.

Approved for use under California Rule 66, THFA<sup>®</sup> can be used in formulations applied to crops before, during, and after harvesting.

### **THFA<sup>®</sup> in Stripping Formulations**

The automotive and metal-fabricating industries use stripping formulations to remove protective coatings, paint, and grime prior to painting and finishing. The use of THFA<sup>®</sup> as a key ingredient in these stripping formulations is quickly growing. THFA<sup>®</sup> is utilized as an activator in hot alkaline stripping baths to remove paint overspray or to remove coatings.

Blends of THFA<sup>®</sup> and furfuryl alcohol, or FACT-1 (ethoxylated furfuryl alcohol), exhibit a synergistic effect that significantly improves the efficiency of alkaline strippers compared to the results obtained by the addition of either product alone.

## **THFA®: The Broad-Spectrum, Safe to Use Cleaner!**

THFA® as a broad-spectrum, safe-to-use cleaner is just beginning to be recognized. THFA® is a key component of cleaning products used in areas where environmental considerations dictate the use of relatively non-toxic, water-miscible, biodegradable solvents. THFA® alone, or in combination with other solvents, is used in such typical applications as:

- floor polish removers
- graffiti remover
- oven cleaners
- industrial cleaners used in the graphic arts industry
- industrial cleaners used in the cleaning of automotive and truck engine parts
- cleaners for the printed circuit board industry
- cleaners for the paper products industry
- cleaners for linoleum, desk tops, and other hard surfaces rug and upholstery cleaners

## **Polymers and Resins**

THFA® is an effective coalescing agent for water emulsion paints. It helps lower the minimum film forming temperature and improves both gloss and freeze-thaw stability. High filler levels can be tolerated in emulsion caulks and sealants containing THFA®. These formulated products are more pressure sensitive and have improved low temperature flexibility.

Tetrahydrofurfuryl acrylate and methacrylate prepared by transesterification of the lower acrylate esters are reactive monomers used in the formulation of ultraviolet light-curable adhesives, coatings, paints, and printing inks. Tetrahydrofurfuryl methacrylate also serves as a reactive curing agent in the peroxide, catalyzed production of nitrile rubber.

THFA® is used for various applications in epoxy resins and is a good solvent for many of the curatives and catalysts used in epoxy formulations. THFA® will accelerate the cure of Bisphenol-A resins with either aliphatic or aromatic amine curatives. It is also a good solvent for boron trifluoride monoethanolamine (BF<sub>3</sub>•MEA). THFA® has been reported to co-react with epoxy groups—becoming an integral part of the system.

## **Deep, Even Dye Penetration: THFA® Esters as Plasticizers and Finishing Agents**

THFA® permits higher dye concentrations and a broader temperature range in solutions because of its high dye solvency which facilitates deep, even penetration of dye into a substrate. For synthetic fibers, this is accomplished through a swelling action. For leather penetration, it is accomplished via the polarities of THFA® and leather. As a leveler, THFA® aids in the attainment of color shade uniformity.

Esters of THFA®, especially tetrahydrofurfuryl oleate, are used as primary and extender-type plasticizers. The oleate ester is a very stable, light-colored plasticizer which improves the low temperature flexibility of vinyl products. It is also used as a carrier to incorporate stabilizers into vinyl resin formulations.

## **Other Applications**

THFA® is used in a broad spectrum of other applications. Many have been commercialized and others are in various stages of development. Examples include:

- Adhesive formulations
- Extractant in the production of lube oils
- Ingredient in lacquers and pharmaceuticals
- Chemical intermediates
- Emulsion polymer additive

## **Typical Analytical Values**

THFA<sup>®</sup> is a high purity product. Typical analytical data are:

Assay.....	%.....	99.0
Water.....	max %.....	0.3
Furfuryl alcohol.....	max %.....	0.1

## **Chemical Properties**

THFA<sup>®</sup> is a stable compound up to its atmospheric boiling point. Degradation may occur at temperatures above the boiling point yielding carbon monoxide and carbon dioxide. In the presence of air, unstabilized THFA<sup>®</sup> will oxidize very slowly to form lactones at ambient temperature. Under neutral conditions, THFA<sup>®</sup> can be distilled without occurrence of color degradations or ring-opening reactions.

THFA<sup>®</sup> undergoes the typical reactions of a primary alcohol, including oxidation, esterification, etherification and dehydration. Dehydration of THFA<sup>®</sup> over alumina produces dihydropyran. THFA<sup>®</sup> can also be converted to a halide or an amine via displacement reactions. The ring is also susceptible to cleavage, yielding a variety of open-chain compounds, some of which may be recycled to form different heterocyclic intermediates.

## **Handling and Storage**

THFA<sup>®</sup> has been produced and used industrially for approximately forty years. When handling and working with THFA<sup>®</sup>, the normal precautions for chemicals of slight toxicity should be observed. This includes avoiding inhalation of the vapors and avoiding contact with the skin and eyes. Always use proper protective equipment and comply with necessary, prudent precautions when storing, handling, or disposing of THFA<sup>®</sup>.

THFA<sup>®</sup> is classified by the Department of Transportation as a combustible liquid which upon ignition gives rise to a NFPA Extinguisher Standard Class B fire. Before handling THFA<sup>®</sup>, read and understand the MSDS which is included with shipments and is available upon request.

Mild steel is the recommended material for container construction for the transport and storage of THFA<sup>®</sup>. Aluminum tank trucks are also acceptable. Steel is used for storage tanks, transfer line valves and fittings, and for drums and tank trucks.

## **Waste**

THFA<sup>®</sup> is not classified as a hazardous waste by the EPA. However, disposal of waste THFA<sup>®</sup> should be in accord with local, state, and federal regulations.

## **Material Compatibility**

THFA<sup>®</sup> is an excellent solvent which affects most elastomers. The preferred material for flange gaskets contacting THFA<sup>®</sup> is Polytetrafluoroethylene (PTFE). PTFE seals and seats are also suggested for gate or ball valves. Standard ANSI centrifugal pumps with single, inside balanced, pusher-type mechanical seals are suggested for transferring THFA<sup>®</sup>. Transfer hoses lined with fluoroplastics are suitable for THFA<sup>®</sup> service. PTFE, FEP (Fluorinated Ethylene Propylene copolymer), and PFA (Perfluoroalkoxyl) are examples of fluoroplastics.

## **Health, Safety and Regulatory**

Exempt from the EPA's tolerance requirement under regulation 40 CFR 180.1001 (c), THFA<sup>®</sup> can be used as a solvent for pesticides on food crops. It is not "photochemically reactive" as defined in California State Regulations Rule 66. THFA<sup>®</sup> is not listed as a carcinogen by NTP or IARC. It is not listed on the hazardous air pollutant (HAP) list or on SARA. THFA is listed on TSCA, ENICS, DSL, ENCS, ECL, PICCS, FEMA GRAS. FIFRA Inert 40 CFR 180.100.

### Availability

THFA<sup>®</sup> is available in bulk tank trucks, in 55 gallon steel drums (475 lbs, 216 Kg) and 5 gallon steel pails (40 lbs, 18 Kg). Samples can be ordered by calling 877-895-PENN or by visiting our web site at [www.pschem.com](http://www.pschem.com)

### Shipping

The DOT code number for THFA<sup>®</sup> is UN1987. 49CFR173.150: Combustible liquids in non-bulk packaging are not regulated by DOT

### Physical Properties of THFA<sup>®</sup>

Molecular weight.....	102.13	Kauri-Butanol value.....	>150
CAS #.....	97-99-4	Specific heat, liquid at 20 °C, cal/g°C.....	0.424
EINCS #.....	202-625-6	Heat of vaporization, cal/g.....	120.6
Appearance.....	colorless liquid	Heat of combustion, const P kcal/mol.....	709.5
Boiling point °C.....	178	Flash point (tag closed cup) °C.....	74
Vapor Pressure at 20 °C, mm Hg.....	0.20	Auto ignition temperature °C.....	282
Freezing point °C.....	below -80	Flammability limits in air	
Specific gravity at 20 °C.....	1.054	lower, volume %.....	1.5
Pounds per gallon at 20 °C.....	8.79	upper, volume %.....	9.7
Refractive index n <sub>D</sub> <sup>20</sup> .....	1.452	Dielectric constant at 23 °C.....	13.6
Surface tension at 25 °C, dynes/cm.....	37	Relative evaporation rate	
Viscosity at 20 °C, cps.....	6.24	(n-butylacetate = 1.00).....	0.03
Hansen solubility parameter			
Nonpolar.....	9.8		
Polar.....	5.0		
Hydrogen bonding.....	7.8		

### **Vapor Pressure**

The vapor pressure of THFA<sup>®</sup> in mm of mercury can be calculated from:

$$\log_{10}(\text{vapor pressure}) = -2586.2(1/^\circ\text{K}) + 8.6227$$

### **Specific Gravity**

The specific gravity (g/cc) of THFA<sup>®</sup> can be calculated from:

$$\text{specific gravity} = -0.0082(^\circ\text{C}) + 1.0719$$

## Solubility of Various Compounds in THFA®

	10 wt. % solids	20 wt. % solids		10 wt. % solids	20 wt. % solids
<b>Acids:</b>			<b>Esters:</b>		
Acetylsalicylic.....	S.....	S	Amyl acetate.....	S.....	S
Anthranilic.....	S.....	S	Butyl acetate.....	S.....	S
Benzoic.....	S.....	S	Cellulose acetate.....	S.....	S
Butyric.....	S.....	S	Diethyl acetate.....	S.....	S
Citric.....	S.....	SS	Diethyl phthalate.....	S.....	S
Cresylic.....	S.....	S	Ethyl acetate.....	S.....	S
Lactic.....	SS.....	S at 120 °C	Ethyl acetoacetate.....	S.....	S
Naphthionic.....	S.....	SS	Methyl acetate.....	S.....	S
Oxalic.....	S.....	SS	<b>Ethers:</b>		
Stearic.....	I (soluble at 100 °C)		Dichloroethyl.....	S.....	S
Sulfanilic.....	I		Diethylene glycol monobutyl....	S.....	S
Tannic.....	I (SS at 130 °C)		Diethylene glycol monoethyl....	S.....	S
Tartaric.....	SS		Ethyl.....	S.....	S
Trichloroacetic.....	S.....	S	Ethylene glycol monobutyl....	S.....	S
Valeric.....	S.....	S	Ethylene glycol monoethyl....	S.....	S
<b>Alcohols:</b>			<b>Halides:</b>		
Benzyl alcohol.....	S.....	S	Benzyl chloride.....	S.....	S
Chloral hydrate.....	S.....	S	Bromobenzene.....	S.....	S
Dinitrophenol.....	S.....	S	Bromoform.....	S.....	S
Ethanol.....	S.....	S	Chloroform.....	S.....	S
Ethylene glycol.....	S.....	S	o-Dichlorobenzene.....	S.....	S
Glycerol.....	S.....	S	p-Dichlorobenzene.....	S.....	SS
Isobutanol.....	S.....	S	Dinitrochlorobenzene.....	S.....	SS
Isopropanol.....	S.....	S	Ethyl bromide.....	S.....	S
1-Naphthol.....	S.....	S	Ethylene chloride.....	S.....	S
2-Naphthol.....	S.....	S	Iodoform.....	S.....	S
Pentanol.....	S.....	S	o-Nitrochlorobenzene.....	S.....	SS
Propanol.....	S.....	S	Tetrachloroethane.....	S.....	S
<b>Aldehydes:</b>			<b>Ketones:</b>		
Benzaldehyde.....	S.....	S	Acetone.....	S.....	S
Crotonaldehyde.....	S.....	S	Anthraquinone.....	I	
Paraformaldehyde.....	S.....	S	Methylethyl ketone.....	S.....	S
<b>Amines:</b>			<b>Oils:</b>		
Aniline.....	S.....	S	Aniline.....	S.....	S
Benzidine.....	S.....	S	Castor.....	I	
Dianisidine.....	S.....	SS	Chinawood.....	I	
Diethyl aniline.....	S.....	S	Coconut.....	I	
Dimethylamine.....	S.....	S	Cottonseed.....	I	
Hexamethylene tetraamine.....	I (SS at 130 °C)		Lard.....	I (S at 120 °C)	
2-Naphthylamine.....	S.....	SS	Linseed.....	I (S at 120 °C)	
m-Phenylenediamine.....	S.....	S	Menhaden.....	I (S at 120 °C)	
Pyridine.....	S.....	S	Neat's-foot.....	I (S at 120 °C)	
o-Toluidine.....	S.....	S	Peanut.....	I (S at 120 °C)	
Triphenylguanidine.....	S.....	SS	Rape-seed.....	I (S at 120 °C)	
Xylidine.....	S.....	S	Sperm.....	I (S at 120 °C)	
<b>Aromatics:</b>			Turkey Red..... S		
Anthracene.....	I (S at 100 °C)		Whale.....	I (S at 120 °C)	
Benzene.....	S.....	S	<b>Miscellaneous Compounds:</b>		
Dinitronaphthalene.....	I (S at 120 °C)		Caffeine.....	I	
Diphenyl.....	S.....	SS	Camphor, monobromo.....	I	
Naphthalene.....	S.....	S	Casein.....	I	
p-Nitrophenol.....	S.....	S	Chloramine.....	I (SS at 130 °C)	
o-Nitrophenol.....	S.....	S	Dextrose.....	I (S at 100 °C)	
p-Nitrotoluene.....	S.....	S	Sodium acetate.....	S	SS
Xylol.....	S.....	S	Sodium benzoate.....	SS at 135 °C	
S=soluble SS=slightly soluble I=insoluble					



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## TETRAHYDROFURFURYL ALCOHOL

Penn Specialty Chemicals, Inc. is a privately owned company with manufacturing operations in Memphis, Tennessee. A line of fine chemicals and solvents derived from furfural are produced at the site.

### **Fine Chemicals**

Furan	Difurylpropane	Methylfuroate
Acetylfuran	Ditetrahydrofurylpropane	Methyltetrahydrofuroate
Furfurylamine	Furoic Acid	Methylfuran
Tetrahydrofurfurylamine	Tetrahydrofuroic Acid	Methyltetrahydrofuran
High purity furfural	Furfuryl Alcohol	Tetrahydrofurfuryl Alcohol

Penn Specialty Chemicals, Inc. also has extensive pilot and production capability for custom manufacturing.

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