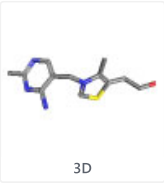
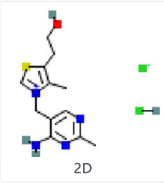


COMPOUND SUMMARY

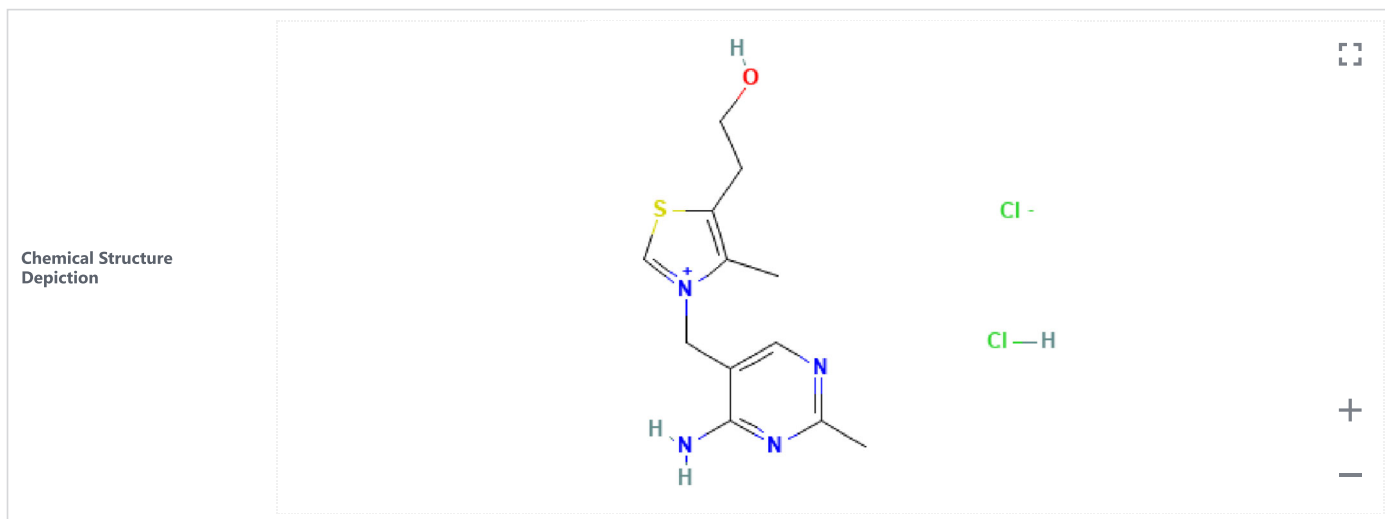
Thiamine hydrochloride

PubChem CID	6202
Structure	 2D3D Find Similar Structures
Chemical Safety	Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	HC ₁₂ H ₁₇ ON ₄ SCl ₂ or C₁₂H₁₈Cl₂N₄OS
Synonyms	THIAMINE HYDROCHLORIDE 67-03-8 Thiamine HCL Aneurine hydrochloride Vitamin B1 hydrochloride More...
Molecular Weight	337.3
Parent Compound	 CID 1130 (Thiamine)
Component Compounds	 CID 1130 (Thiamine)  CID 313 (Hydrochloric Acid)
Dates	Modify 2022-11-26 Create 2005-03-27
Thiamine Hydrochloride is the hydrochloride salt form of thiamine, a vitamin essential for aerobic metabolism, cell growth, transmission of nerve impulses and acetylcholine synthesis. Upon hydrolysis, thiamine hydrochloride is phosphorylated by thiamine diphosphokinase to form active thiamine pyrophosphate (TPP), also known as cocarboxylase. TPP is a coenzyme for many enzymatic activities involving fatty acid, amino acid and carbohydrate metabolism. ► NCI Thesaurus (NCIt) Thiamine hydrochloride is a hydrochloride obtained by combining thiamine chloride with one molar equivalent of hydrochloric acid. It has a role as an insect repellent. It is a vitamin B1 and a hydrochloride. It contains a thiamine(2+). ► ChEBI	

1 Structures



1.1 2D Structure



► PubChem

1.2 3D Conformer



3D Conformer of Parent

► PubChem

2 Names and Identifiers



2.1 Computed Descriptors



2.1.1 IUPAC Name



2-[3-[(4-amino-2-methylpyrimidin-5-yl)methyl]-4-methyl-1,3-thiazol-3-ium-5-yl]ethanol;chloride;hydrochloride

Computed by Lexichem TK 2.7.0 (PubChem release 2021.05.07)

► PubChem

2.1.2 InChI



InChI=1S/C12H17N4OS.2ClH/c1-8-11(3-4-17)18-7-16(8)6-10-5-14-9(2)15-12(10)13;/h5,7,17H,3-4,6H2,1-2H3,(H2,13,14,15);2*1H/q+1,;/p-1

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

► PubChem

2.1.3 InChIKey



DPJRMOMPQZCRJU-UHFFFAOYSA-M

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

► PubChem

2.1.4 Canonical SMILES



CC1=C(SC=[N+])1CC2=CN=C(N=C2N)C)CCO.Cl.[Cl-]

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

► PubChem

2.2 Molecular Formula



HC12H17ON4SCl2

► Wikipedia

C12H18Cl2N4OS

Computed by PubChem 2.1 (PubChem release 2021.05.07)

► PubChem

2.3 Other Identifiers



2.3.1 CAS



67-03-8

► CAS Common Chemistry; ChemIDplus; DTP/NCI; EPA Chemicals under the TSCA; EPA DSSTox; European Chemicals Agency (ECHA); FDA Global Substance Registration System (GSRS)

59-43-8

► Hazardous Substances Data Bank (HSDB)

2.3.2 Deprecated CAS



63-66-1, 70732-86-4, 108631-50-1, 2173536-98-4, 2227489-38-3

► ChemIDplus

108631-50-1, 63-66-1, 70732-86-4

2.3.3 European Community (EC) Number

200-641-8

European Chemicals Agency (ECHA)

2.3.4 NSC Number

36226

DTP/NCI

2.3.5 UNII

M57Z600ESP

FDA Global Substance Registration System (GSRS)

2.3.6 JECFA Number

1030

Joint FAO/WHO Expert Committee on Food Additives (JECFA)

2.3.7 FEMA Number

3322

Flavor and Extract Manufacturers Association (FEMA); Joint FAO/WHO Expert Committee on Food Additives (JECFA)

2.3.8 DSSTox Substance ID

DTXSID0040622

EPA DSSTox

2.3.9 Wikipedia

Thiamine hydrochloride

Wikipedia

2.3.10 Wikidata

Q27121486

Wikidata

2.3.11 NCI Thesaurus Code

C48025

NCI Thesaurus (NCIt)

2.3.12 RXCUI

235355

NLM RxNorm Terminology

2.4 Synonyms

?

2.4.1 MeSH Entry Terms

?

thiamine chloride hydrochloride
thiamine hydrochloride

► Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms

?

THIAMINE HYDROCHLORIDE	Begiolan	Thiavit	Hybee	Usaf cb-20	NSC-36226
67-03-8	Benerva	Tiamidon	Apate drops	FEMA No. 3322	3-[(4-amino-2-methylpyrimidin-5-yl)methy
Thiamine HCL	Bethiazine	Tiaminal	Lixa-beta	Vitamin B hydrochloride	Thiamine, monohydrochloride
Aneurine hydrochloride	Bevitex	Trophite	Thiamin chloride	Thiaminium chloride hydrochloride	Thiamine HCl (Vitamin B1)
Vitamin B1 hydrochloride	Bevitine	Vinothiam	Thiaminum hydrochloricum	thiamine(2+) dichloride	Vitamin B1 (Thiamine HCl)
Clotiamina	Bithiamin	Vitaneuron	Vetalin S	Thiamine monohydrochloride	67-03-8 (HCl salt)
Thiamine chloride hydrochloride	Bivatin	Bedome	Thiaminium chloride	MFCD00012780	CHEBI:49105
Eskapen	Eskapen	Beuion	Betaxin	Betabion	M572600E5P
Betalin S	Metabolin	Bivita	Thiadoxine	Betamin	CAS-67-03-8
vitamin B1	Slowten	Berin	Bequin	Biamine	NCGC00017013-01
Thiamine dichloride	Thiaminal	Bewon	Thiamin hydrochloride	Vitamin b(sub 1) hydrochloride	2-[3-[(4-amino-2-methylpyrimidin-5-yl)me
Beatine	Thiamol	Biuno	Betabion hydrochloride	Thiamine (hydrochloride)	2-[3-[(4-amino-2-methylpyrimidin-5-yl)me

► PubChem

3 Chemical and Physical Properties



3.1 Computed Properties



Property Name	Property Value	Reference
Molecular Weight	337.3	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Hydrogen Bond Donor Count	3	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Hydrogen Bond Acceptor Count	6	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Rotatable Bond Count	4	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Exact Mass	336.0578378	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Monoisotopic Mass	336.0578378	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Topological Polar Surface Area	104 Å²	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Heavy Atom Count	20	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	269	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	0	Computed by PubChem
Undefined Atom Stereocenter Count	0	Computed by PubChem
Defined Bond Stereocenter Count	0	Computed by PubChem
Undefined Bond Stereocenter Count	0	Computed by PubChem
Covalently-Bonded Unit Count	3	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2021.05.07)

PubChem

3.2 Experimental Properties



3.2.1 Physical Description

Small white to yellowish crystals or crystalline powder; slight characteristic odour reminiscent of **thiazole**
Solid with a mild **thiazole** odor; [Merck Index] White to light yellow crystalline powder; Hygroscopic; [Alfa Aesar MSDS]

Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

Joint FAO/WHO Expert Committee on Food Additives (JECFA)

3.2.2 Color/Form

Crystals from water

Lewis, R.L. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004, p. 3441

Hazardous Substances Data Bank (HSDB)

3.2.3 Odor

SLIGHT, CHARACTERISTIC

Osol, A. and J.E. Hoover, et al. (eds.). Remington's Pharmaceutical Sciences. 15th ed. Easton, Pennsylvania: Mack Publishing Co., 1975, p. 962

Hazardous Substances Data Bank (HSDB)

3.2.4 Melting Point

164 °C

Lide, D.R. CRC Handbook of Chemistry and Physics 88TH Edition 2007-2008. CRC Press, Taylor & Francis, Boca Raton, FL. 2007, p. 3-482

Hazardous Substances Data Bank (HSDB)

MP: 248 °C, DECOMP /HYDROCHLORIDE/

Fenaroli's Handbook of Flavor Ingredients. Volume 2. Edited, translated, and revised by T.E. Furtu and N. Bellanca. 2nd ed. Cleveland: The Chemical Rubber Co., 1975, p. 562

► Hazardous Substances Data Bank (HSDB)

3.2.5 Solubility



SLIGHTLY SOL IN ALC & **CHLOROFORM** /MONONITRATE/

Osol, A. and J.E. Hoover, et al (eds.). Remington's Pharmaceutical Sciences. 15th ed. Easton, Pennsylvania: Mack Publishing Co., 1975, p. 962

► Hazardous Substances Data Bank (HSDB)

MONONITRATE IS MUCH LESS SOL IN **WATER** THAN HYDROCHLORIDE

Furtu, T.E. (ed.). CRC Handbook of Food Additives. 2nd ed. Cleveland: The Chemical Rubber Co., 1972, p. 104

► Hazardous Substances Data Bank (HSDB)

In **water**, approximately 5.0X10+5 mg/L, temp not specified

Budavari, S. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 1996.

► Hazardous Substances Data Bank (HSDB)

Soluble in **water**, **propylene glycol**; insoluble in ether, **benzene**, **hexane**, **chloroform**

► Joint FAO/WHO Expert Committee on Food Additives (JECFA)

Slightly soluble (in **ethanol**)

► Joint FAO/WHO Expert Committee on Food Additives (JECFA)

3.2.6 Vapor Pressure



1.8X10-10 mm Hg at 25 °C (est)

US EPA: Estimation Program Interface (EPI) Suite. Ver. 4.0. Jan, 2009. Available from, as of Feb 16, 2010: <https://www.epa.gov/oppt/exposure/pubs/episuite.htm>

► Hazardous Substances Data Bank (HSDB)

3.2.7 Stability/Shelf Life



Stable under normal storage conditions; it is degraded in neutral and alkaline solutions (even at room temp)

Furtu, T.E. (ed.). CRC Handbook of Food Additives. 2nd ed. Cleveland: The Chemical Rubber Co., 1972, p. 89

► Hazardous Substances Data Bank (HSDB)

Mononitrate is less hygroscopic and hence is more stable than the hydrochloride /Mononitrate and hydrochloride salts/

Furtu, T.E. (ed.). CRC Handbook of Food Additives. 2nd ed. Cleveland: The Chemical Rubber Co., 1972, p. 104

► Hazardous Substances Data Bank (HSDB)

Stability is excellent in low pH fruit drinks, eg, losses in drinks are 6% after 12 mo at room temp

Furtu, T.E. (ed.). CRC Handbook of Food Additives. 2nd ed. Cleveland: The Chemical Rubber Co., 1972, p. 105

► Hazardous Substances Data Bank (HSDB)

Stability in frozen drink concentrate is excellent

Furtu, T.E. (ed.). CRC Handbook of Food Additives. 2nd ed. Cleveland: The Chemical Rubber Co., 1972, p. 105

► Hazardous Substances Data Bank (HSDB)

For more Stability/Shelf Life (Complete) data for **Vitamin B1** (9 total), please visit the [HSDB record page](#).

► Hazardous Substances Data Bank (HSDB)

3.2.8 Decomposition



When heated to decomposition it emits very toxic fumes of **/nitric oxide/**, **/sulfur oxide/**, and **/chlorine/**.

Lewis, R.J. Sr. (ed) *Sax's Dangerous Properties of Industrial Materials*. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 3441

► [Hazardous Substances Data Bank \(HSDB\)](#)

3.2.9 Other Experimental Properties



Monoclinic plates in rosette-like clusters. Slight [thiazole](#) odor; bitter taste; decomposes at 248 °C. One gram dissolves in approximately 1 mL [water](#), 18 mL [glycerol](#), 100 mL 95% alcohol, 315 mL absolute alcohol; more soluble in [methanol](#). Soluble in [propylene glycol](#). Practically insoluble in ether, [benzene](#), [hexane](#), [chloroform](#). pH of 1% wt/vol solution in [water](#) 3.13; pH of 0.1% wt/vol solution in [water](#) 3.58. On exposure to air of average humidity, the vitamin absorbs an amount of [water](#) corresponding to nearly one mole, forming a [hydrate](#).

O'Neil, M.J. (ed.). *The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals*. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 1598

► [Hazardous Substances Data Bank \(HSDB\)](#)

HYGROSCOPIC; NUT-LIKE ODOR /HYDROCHLORIDE/

Sax, N.I. *Dangerous Properties of Industrial Materials*. 5th ed. New York: Van Nostrand Reinhold, 1979., p. 1027

► [Hazardous Substances Data Bank \(HSDB\)](#)

READILY SPLIT BY [SULFITE](#) INTO ITS [PYRIMIDINE](#) & [THIAZOLE](#) CONSTITUENTS

Furia, T.E. (ed.). *CRC Handbook of Food Additives*. 2nd ed. Cleveland: The Chemical Rubber Co., 1972., p. 89

► [Hazardous Substances Data Bank \(HSDB\)](#)

Crystals. MP: 196-200 °C, decomposes; practically nonhygroscopic; pKa = 4.9. Solubility in [water](#) (g/100 mL): 2.7 (25 °C); approximately 30 (100 °C). pH of 2% aqueous solution 6.5 to 7.1, more stable than the hydrochloride; suitable for enrichment of flours and feeds, multivitamin preparations /Mononitrate/

O'Neil, M.J. (ed.). *The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals*. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 1598

► [Hazardous Substances Data Bank \(HSDB\)](#)

SMALL WHITE CRYSTALS OR CRYSTALLINE POWDER /HYDROCHLORIDE/

Osol, A. and J.E. Hoover, et al. (eds.). *Remington's Pharmaceutical Sciences*. 15th ed. Easton, Pennsylvania: Mack Publishing Co., 1975., p. 961

► [Hazardous Substances Data Bank \(HSDB\)](#)

Thiamine hydrochloride in the dry state is stable. Acidic solutions having a pH below 5.5 preferably from 5.0 to 3.5 are also relatively stable. Alkalies destroy it. It is precipitated from solution by several of the alkaloidal reagents such as [mercuric chloride](#), [iodine](#), [picric acid](#), tannin, and [Mayer's reagent](#). It is sensitive to both oxidizing and reducing agents. /Hydrochloride/

Chase et al; *Remington's Pharmaceutical Sciences* 14th ed. Mack Publ Co. Easton, PA p. 1040 (1970)

► [Hazardous Substances Data Bank \(HSDB\)](#)

For more Other Experimental Properties (Complete) data for [Vitamin B1](#) (6 total), please visit the [HSDB record page](#).

► [Hazardous Substances Data Bank \(HSDB\)](#)

3.2.10 Chemical Classes



Biological Agents -> Vitamins and Derivatives

► [Haz-Map, Information on Hazardous Chemicals and Occupational Diseases](#)

4 Spectral Information

4.1 1D NMR Spectra

4.1.1 1H NMR Spectra

3958	Spectra ID
JEOL	Instrument Type
400 MHz	Frequency
DMSO-d6	Solvent
10.01:350.00, 2.54:979.00, 2.58:1000.00, 3.06:161.00, 3.07:128.00, 3.08:284.00, 3.09:169.00, 3.42:170.00, 3.64:188.00, 3.66:302.00, 3.67:166.00, 5.64:26.00, 5.64:27.00, 5.64:29.00, 5.64:30.00, 5.64:33.00, 5.67:443.00, 8.39:312.00, 9.28:114.00	Shifts [ppm]:Intensity
Thumbnail	

Human Metabolome Database (HMDB)

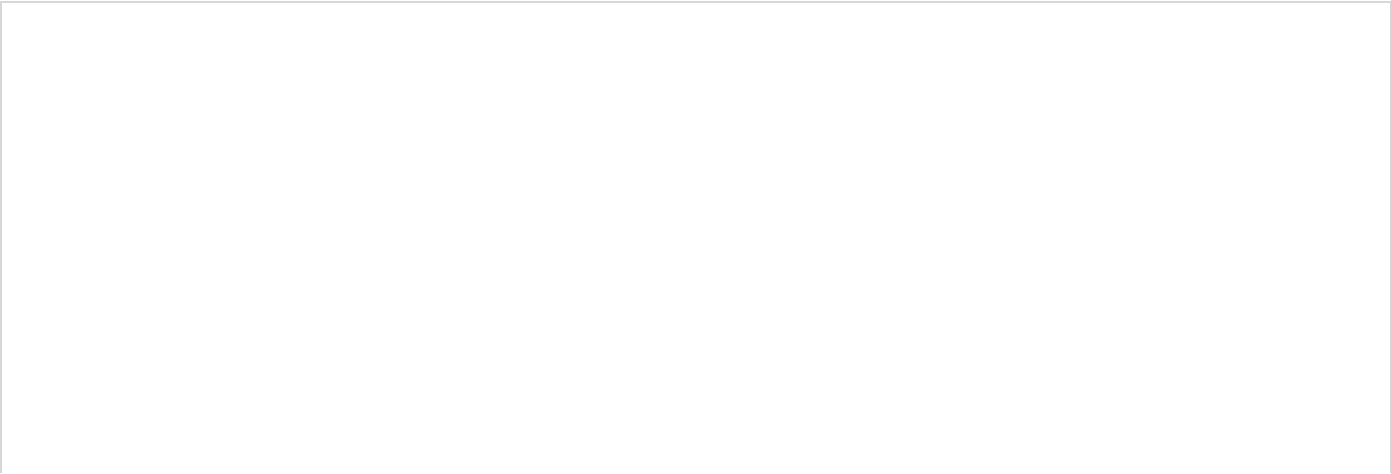
4.1.2 13C NMR Spectra

4240	Spectra ID
50.18 MHz	Frequency
D2O	Solvent
107.06:455.00, 12.09:938.00, 137.48:567.00, 143.81:497.00, 146.48:828.00, 154.70:39.00, 155.36:44.00, 155.60:81.00, 156.02:36.00, 163.95:306.00, 164.66:418.00, 22.22:911.00, 30.26:959.00, 50.97:844.00, 61.28:1000.00	Shifts [ppm]:Intensity
Thumbnail	

Human Metabolome Database (HMDB)

Source of Sample	MCB Manufacturing Chemists, Norwood, Ohio
Copyright	Copyright © 1980, 1981-2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

► SpectraBase



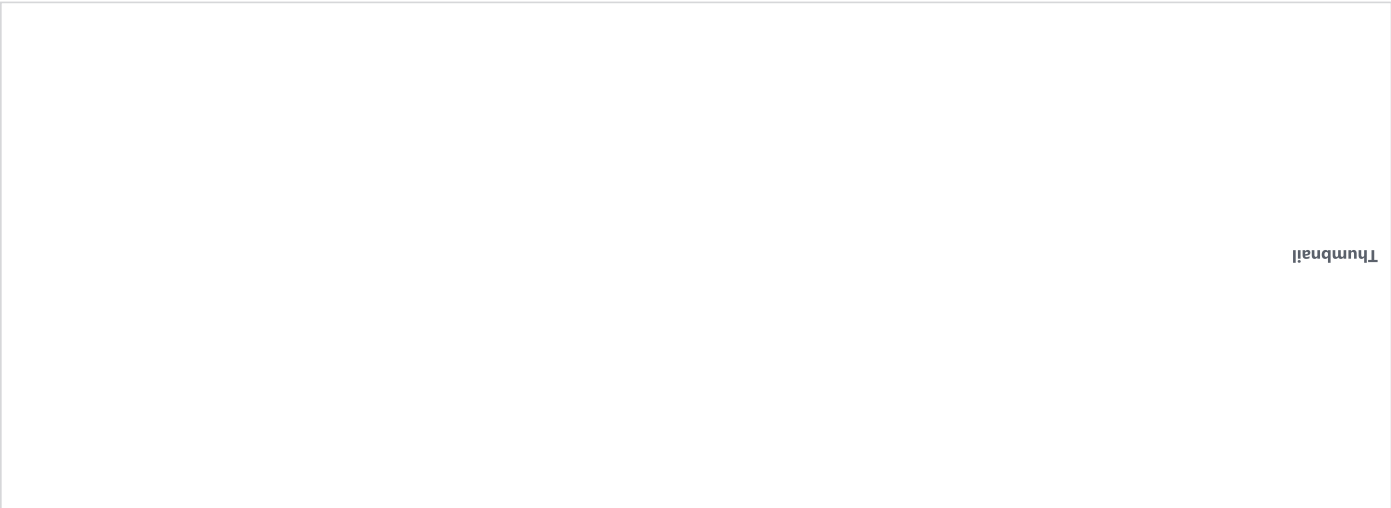
4.2 Mass Spectrometry



4.2.1 GC-MS



Source of Spectrum	B4-0-0-0
Copyright	Copyright © 2020-2021 John Wiley & Sons, Inc. All Rights Reserved.



► SpectraBase

4.3 UV Spectra



MAX ABSORPTION (WATER, PH 8): 235 NM (LOG E= 4.1); 268 NM (LOG E= 3.9); SADTLER REF NUMBER: 324 (IR, PRISM); 123 (UV) /HYDROCHLORIDE/
West, R.C. (ed.), Handbook of Chemistry and Physics. 60th ed. Boca Raton, Florida: CRC Press Inc., 1979, p. C-543
► Hazardous Substances Data Bank (HSDB)

4.3.1 UV-VIS Spectra



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Thumbnail	



► SpectraBase

4.4 IR Spectra



4.4.1 FTIR Spectra



Technique	KBr WAFER
Source of Sample	Fluka Chemie AG, Buchs, Switzerland
Copyright	Copyright © 1980, 1981-2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

► SpectraBase

Technique	KBr WAFER
Source of Sample	Fluka Chemie AG, Buchs, Switzerland
Copyright	Copyright © 1980, 1981-2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

► SpectraBase

4.5 Raman Spectra



Technique	FT-Raman
-----------	----------

Source of Spectrum	Forensic Spectral Research
Source of Sample	Supelco, Sigma-Aldrich
Catalog Number	47858
Lot Number	LB61003
Copyright	Copyright © 2012-2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

► SpectraBase

4.6 Other Spectra

WHEN EXPOSED TO AIR, ANHYD PRODUCT RAPIDLY ABSORBS ABOUT 4% OF **WATER**; SOLN ARE ACID TO LITMUS PAPER. PH (1 IN 100 SOLN) BETWEEN 2.7 &

3.4; ACIDIC SOLN HAVE PH BELOW 5.5; ALKALIES DESTROY IT /HYDROCHLORIDE/

Osol, A. and J.E. Hoover, et al (eds). Remington's Pharmaceutical Sciences. 15th ed. Easton, Pennsylvania: Mack Publishing Co., 1975, p. 961

► Hazardous Substances Data Bank (HSDB)

► PubChem

CID 1130 (Thiamine)

► PubChem



CID 1130 (Thiamine)

CID 313 (Hydrochloric Acid)

► PubChem

Same Connectivity	5 Records
Same Parent, Connectivity	134 Records
Same Parent, Exact	121 Records
Mixtures, Components, and Neutralized Forms	2 Records
Similar Compounds	264 Records

► PubChem

Same	173 Records
------	-------------

► PubChem

5.5.2 Substances by Category

▶ PubChem

5.6 Entrez Crosslinks

PubMed	1 Record
--------	----------

▶ PubChem

5.7 Associated Chemicals

Thiamine disulfide;67-16-3

▶ Hazardous Substances Data Bank (HSDB)

Thiamine hydrochloride;67-03-8

▶ Hazardous Substances Data Bank (HSDB)

Thiamine mononitrate;532-43-4

▶ Hazardous Substances Data Bank (HSDB)

Thiamine tetrahydrofurfuryl disulfide;804-30-8

▶ Hazardous Substances Data Bank (HSDB)

6 Chemical Vendors



► PubChem

7 Drug and Medication Information



7.1 FDA Orange Book



FDA Orange Book

7.2 FDA National Drug Code Directory



National Drug Code (NDC) Directory

THIAMINE HYDROCHLORIDE is an active ingredient in 42 products including: 'ADULT INFUVITE MULTIPLE VITAMINS', 'B COMPLEX MIX SYSTEM FORMULA', and 'BIO CO-ENZYME PHASE'.

National Drug Code (NDC) Directory

7.3 Drug Labels for Ingredients



Label Information	Total 4 labels
Drug Ingredient	ALPHA-TOCOPHEROL ACETATE; ASCORBIC ACID; BIOTIN; CHOLECALCIFEROL; CYANOCOBALAMIN; DEXPANTHENOL; FOLIC ACID; NIACINAMIDE; PYRIDOXINE HYDROCHLORIDE; RIBOFLAVIN 5'-PHOSPHATE SODIUM; THIAMINE HYDROCHLORIDE; VITAMIN A PALMITATE; VITAMIN K
NDC Code(s)	54643-5649-1, 54643-5650-2, 54643-7862-1, 54643-7874-2, 54643-9007-1, 54643-9015-2
Packagers	Sandoz Canada Inc; Sandoz Manufacturing Inc

DailyMed

Label Information	Total 220 labels
Drug Ingredient	THIAMINE HYDROCHLORIDE

NDC Code(s)	0178-0716-90, 0178-0864-30, 0178-0891-30, 0178-0893-30, 0404-9963-02, 0641-6228-01, 0641-6228-25, 0642-0072-12, 0642-0075-30, 0642-0076-30 ... total 197.
Packagers	A-S Medication Solutions; Acella Pharmaceuticals, LLC; Agile RX; Agri Laboratories, Inc.; Akron Pharma; Allegis Pharmaceuticals, LLC; Amneal Pharmaceuticals LLC; Apace Packaging, LLC; Arize Supplements, LLC; Aspen Veterinary Resources, Ltd. ... total 107.

► [DailyMed](#)

7.4 Clinical Trials

?

↗

7.4.1 ClinicalTrials.gov

?

↗

► [ClinicalTrials.gov](#)

7.4.2 EU Clinical Trials Register

?

↗

► [EU Clinical Trials Register](#)

7.5 Therapeutic Uses

?

↗

Thiamine is used to prevent and to treat **thiamine** deficiency syndromes including beriberi, Wernicke's encephalopathy syndrome, delirium, and peripheral neuritis associated with pellagra or neuritis of pregnancy (if associated with severe vomiting).

American Society of Health System Pharmacists; AHFS Drug Information 2009. Bethesda, MD. (2009)

► [Hazardous Substances Data Bank \(HSDB\)](#)

Although **thiamine** has not been shown by well-controlled trials to have any therapeutic value, the drug has been used for the management of poor appetite, ulcerative colitis, chronic diarrhea, other GI disorders, and the cerebellar syndrome. **Thiamine** has also been used orally as an insect repellent, but there is a lack of adequate evidence to establish the efficacy of **thiamine** for this use.

American Society of Health System Pharmacists; AHFS Drug Information 2009. Bethesda, MD. (2009)

► [Hazardous Substances Data Bank \(HSDB\)](#)

Low plasma **thiamine** concentrations have been found in patients with type 1 and type 2 diabetes mellitus. In a small placebo-controlled study, **benfotiamine** /a related **vitamin B1** substance/ 100 mg given four times daily by mouth significantly improved neuropathic pain in patients with diabetic polyneuropathy.

/Benfotiamine/

Sweetman SC (ed), Martindale: The Complete Drug Reference. London: Pharmaceutical Press (2009), p. 1976-7.

► [Hazardous Substances Data Bank \(HSDB\)](#)

/This study assessed/ the effect of **thiamine** repletion on **thiamine** status, functional capacity, and left ventricular ejection fraction (LVEF) in patients with moderate to severe congestive heart failure (CHF) who had received **furosemide** in doses of 80 mg/d or more for at least 3 months. PATIENTS AND METHODS: Thirty patients were randomized to 1 week of double-blind inpatient therapy with either iv **thiamine** 200 mg/d or placebo (n = 15 each). All previous drugs were continued. Following discharge, all 30 patients received oral **thiamine** 200 mg/d as outpatients for 6 weeks. **Thiamine** status was determined by the erythrocyte **thiamine-pyrophosphate** effect (TPPE). LVEF was determined by echocardiography. RESULTS: TPPE, diuresis, and LVEF were unchanged with iv placebo. After iv **thiamine**, TPPE decreased (11.7% +/- 6.5% to 5.4% +/- 3.2%; P < 0.01). LVEF increased (0.28 +/- 0.11 to 0.32 +/- 0.09; P < 0.05), as did diuresis (1,731 +/- 800 mL/d to 2,389 +/- 752 mL/d; P < 0.02), and sodium excretion (84 +/- 52 mEq/d to 116 +/- 83 mEq/d, P < 0.05). In the 27 patients completing the full 7-week intervention, LVEF rose by 22% (0.27 +/- 0.10 to 0.33 +/- 0.11, P < 0.01). CONCLUSIONS: Thiamine repletion can improve left ventricular function and biochemical evidence of thiamine deficiency in some patients with moderate-to-severe CHF who are receiving longterm furosemide therapy.

PMID:7733128

Shimon I et al; Am J Med 98 (5): 485-90 (1995).

► [Hazardous Substances Data Bank \(HSDB\)](#)

For more Therapeutic Uses (Complete) data for **Vitamin B1** (11 total), please visit the [HSDB record page](#).

► [Hazardous Substances Data Bank \(HSDB\)](#)

7.6 Drug Warnings



Serious hypersensitivity/anaphylactic reactions can occur, especially after repeated administration. Deaths have resulted from IV or IM administration of **thiamine**.

Novak, K.M. (ed.). Drug Facts and Comparisons 2008 Edition. Wolters Kluwer Health. St. Louis, Missouri 2008., p. 18

► [Hazardous Substances Data Bank \(HSDB\)](#)

Anaphylaxis as an adverse systemic reaction to **thiamine** (**vitamin B1**) has been described in the literature since 1938. Although its precise mechanism is still uncertain, the reaction appears to involve immediate type hypersensitivity and to be exclusively related to parenteral administration...

PMID:9846348

Morinville V et al; Schweiz Med Wochenschr 128 (44): 1743-4 (1998).

► [Hazardous Substances Data Bank \(HSDB\)](#)

Anaphylaxis. There have been occasional reports of serious and even fatal responses to the parenteral administration of **thiamin**. The clinical characteristics have strongly suggested an anaphylactic reaction. Symptoms associated with **thiamin**-induced anaphylaxis include anxiety, pruritus, respiratory distress, nausea, abdominal pain, and shock, sometimes progressing to death.

NAS, Food and Nutrition Board, Institute of Medicine; Dietary Reference Intakes for Thiamin, Riboflavin, Niacin, Vitamin B6, Folate, Vitamin B12, Pantothenic Acid, Biotin, and Choline. National Academy Press, Washington, D.C., pg. 81, 1998. Available from, as of March 2, 2010: <https://www.nap.edu/catalog/6015.html>

► [Hazardous Substances Data Bank \(HSDB\)](#)

Adverse reactions with **thiamine** are rare, but hypersensitivity reactions have occurred, mainly after parenteral doses. These reactions have ranged in severity from very mild to, very rarely, fatal anaphylactic shock ... The UK Committee on Safety of Medicines had received, between 1970 and July, 1988, 90 reports of adverse reactions associated with the use of an injection containing high doses of vitamins B and C. The most frequent reactions were anaphylaxis (41 cases, including 2 fatalities), dyspnea or bronchospasm (13 cases), and rash or flushing (22 cases); 78 of the reactions occurred during, or shortly after, intravenous injection and the other 12 after intramuscular injection. They recommended that parenteral treatment be used only when essential, and that, when given, facilities for treating anaphylaxis should be available. They also recommended that, when the intravenous route was used, the injection be given slowly (over 10 minutes). Various authors have noted that parenteral treatment is essential for the prophylaxis and treatment of Wernicke's encephalopathy. However, further reports of anaphylaxis to parenteral **thiamine** have since been described, including one with a fatal outcome.

Sweetman SC (ed), Martindale: The Complete Drug Reference. London: Pharmaceutical Press (2009), p. 1976.

► [Hazardous Substances Data Bank \(HSDB\)](#)

For more Drug Warnings (Complete) data for **Vitamin B1** (15 total), please visit the [HSDB record page](#).

► [Hazardous Substances Data Bank \(HSDB\)](#)

8 Food Additives and Ingredients



8.1 Food Additive Classes

Flavoring Agents

► EU Food Improvement Agents; Joint FAO/WHO Expert Committee on Food Additives (JECFA)

JECFA Functional Classes

Flavouring Agent -> FLAVOURING_AGENT;

► Joint FAO/WHO Expert Committee on Food Additives (JECFA)

8.2 FDA Substances Added to Food



Substance	THIAMINE HYDROCHLORIDE
Used for (Technical Effect)	NUTRIENT SUPPLEMENT
Document Number (21 CFR)	184.1875

► FDA Center for Food Safety and Applied Nutrition (CFSAN)

8.3 Evaluations of the Joint FAO/WHO Expert Committee on Food Additives - JECFA



Chemical Name	ANEURINE HYDROCHLORIDE
Evaluation Year	2002
ADI	No safety concern at current levels of intake when used as a flavouring agent
Report	TRS 913-JECFA 59/65
Tox Monograph	FAS 50-JECFA 59/265

► Joint FAO/WHO Expert Committee on Food Additives (JECFA)

Chemical Name	THIAMINE HYDROCHLORIDE
Evaluation Year	2002
ADI	No safety concern at current levels of intake when used as a flavouring agent
Report	TRS 913-JECFA 59/65
Tox Monograph	FAS 50-JECFA 59/265

► Joint FAO/WHO Expert Committee on Food Additives (JECFA)

Chemical Name	VITAMIN B1 HYDROCHLORIDE
Evaluation Year	2002
ADI	No safety concern at current levels of intake when used as a flavouring agent
Report	TRS 913-JECFA 59/65
Tox Monograph	FAS 50-JECFA 59/265

► Joint FAO/WHO Expert Committee on Food Additives (JECFA)

9 Pharmacology and Biochemistry



9.1 FDA Pharmacological Classification



Non-Proprietary Name	METABOLIN
Pharmacological Classes	Amino Acids [CS]; Blood Coagulation Factor [EPC]; Calcium [CS]; Calculi Dissolution Agent [EPC]; Cations, Divalent [CS]; Increased Coagulation Factor Activity [PE]; Increased Large Intestinal Motility [PE]; Inhibition Large Intestine Fluid/Electrolyte Absorption [PE]; Inhibition Small Intestine Fluid/Electrolyte Absorption [PE]; Magnesium Ion Exchange Activity [MoA]; Osmotic Activity [MoA]; Osmotic Laxative [EPC]; Potassium Compounds [CS]; Potassium Salt [EPC]; Stimulation Large Intestine Fluid/Electrolyte Secretion [PE]; Amino Acid [EPC]

► [National Drug Code \(NDC\) Directory](#)

9.2 Bionecessity



Persons who may have increased needs for [thiamin](#) include those being treated with hemodialysis or peritoneal dialysis, individuals with malabsorption syndrome, women carrying more than one fetus, and lactating women who are nursing more than one infant.

NAS, Food and Nutrition Board, Institute of Medicine; Dietary Reference Intakes for Thiamin, Riboflavin, Niacin, Vitamin B6, Folate, Vitamin B12, Pantothenic Acid, Biotin, and Choline. National Academy Press, Washington, D.C., pg. 79, 1998. Available from, as of March 2, 2010: <https://www.nap.edu/catalog/6015.html>

► [Hazardous Substances Data Bank \(HSDB\)](#)

Heavy exercise under certain conditions may increase the requirement for [thiamin](#) as well as other vitamins, but the observations on the effects of physical activity on the [thiamin](#) requirement have been inconsistent, the effects small, and the experimental conditions highly variable. ... Under normal conditions, physical activity does not appear to influence [thiamin](#) requirements to a substantial degree. However, those who are engaged in physically demanding occupations or who spend much time training for active sports may require additional [thiamin](#).

NAS, Food and Nutrition Board, Institute of Medicine; Dietary Reference Intakes for Thiamin, Riboflavin, Niacin, Vitamin B6, Folate, Vitamin B12, Pantothenic Acid, Biotin, and Choline. National Academy Press, Washington, D.C., pg. 63-64, 1998. Available from, as of March 2, 2010: <https://www.nap.edu/catalog/6015.html>

► [Hazardous Substances Data Bank \(HSDB\)](#)

It has been observed that during periods of starvation such as in war, larger individuals present signs of beriberi more rapidly than do those with smaller body builds, indicating their greater needs for [thiamin](#) and other energy-related nutrients.

NAS, Food and Nutrition Board, Institute of Medicine; Dietary Reference Intakes for Thiamin, Riboflavin, Niacin, Vitamin B6, Folate, Vitamin B12, Pantothenic Acid, Biotin, and Choline. National Academy Press, Washington, D.C., pg. 63, 1998. Available from, as of March 2, 2010: <https://www.nap.edu/catalog/6015.html>

► [Hazardous Substances Data Bank \(HSDB\)](#)

[Thiamin](#) ... functions as a coenzyme in the metabolism of carbohydrates and branched-chain amino acids ... The adult requirements for [thiamin](#) are based on the amount of the vitamin needed to achieve and maintain normal erythrocyte transketolase activity, while avoiding excessive [thiamin](#) excretion ... Dietary Reference Intakes (DRIs) are listed by life stage group in the table.

Table: DRI Values for [Thiamin](#) by Life Stage Group mg/day

Life Stage Group	Estimated Average Requirement	Recommended Dietary Allowance	Adequate Intake
0-6 mo			0.2
7-12 mo			0.3
1-3 yr	0.4 (male& female)	0.5 (male & female)	
4-8 yr	0.5 (male & female)	0.6 (male & female)	
9-13 yr	0.7 (male & female)	0.9 (male & female)	
14-18 yr	1.0 (male) 0.9 (female)	1.2 (male) 1.0 (female)	
19-30 yr	1.0 (male) 0.9 female)	1.2 (male) 1.1 (female)	
31-50 yr	1.0 (male) 0.9 (female)	1.2 (male) 1.1 (female)	
51-70 yr	1.0 (male) 0.9 (female)	1.2 (male) 1.1 (female)	
> 70 yr	1.0 (male) 0.9 (female)	1.2 (male) 1.1 (female)	
Pregnancy			
< or = 18 yr	1.2	1.4	
19-50 yr	1.2	1.4	
Lactation			
< or = 18 yr	1.2	1.4	
19-50 yr	1.2	1.4	

Otten JJ, Hellwig JP, Meyers LD, eds; Dietary Reference Intakes: The Essential Guide to Nutrient Requirements, Washington, DC: The National Academies Press, 2006, p.280-1

► [Hazardous Substances Data Bank \(HSDB\)](#)

For more Bionecessity (Complete) data for **Vitamin B1** (43 total), please visit the [HSDB record page](#).

► [Hazardous Substances Data Bank \(HSDB\)](#)

9.3 Absorption, Distribution and Excretion



Absorption of **thiamin** occurs mainly in the jejunum. At low concentrations of **thiamin**, absorption occurs by an active transport system that involves phosphorylation; at higher concentrations, absorption occurs by passive diffusion. Only a small percentage of a high dose of **thiamin** is absorbed, and elevated serum values result in active urinary excretion of the vitamin.

Otten JJ, Hellwig JP, Meyers LD, eds; *Dietary Reference Intakes: The Essential Guide to Nutrient Requirements*, Washington, DC: The National Academies Press, 2006, p. 281

► [Hazardous Substances Data Bank \(HSDB\)](#)

Thiamin is transported in blood in both erythrocytes and plasma and is excreted in the urine.

Otten JJ, Hellwig JP, Meyers LD, eds; *Dietary Reference Intakes: The Essential Guide to Nutrient Requirements*, Washington, DC: The National Academies Press, 2006, p.281

► [Hazardous Substances Data Bank \(HSDB\)](#)

Thiamine is absorbed from the small intestine and is phosphorylated in the intestinal mucosa.

Furia, T.E. (ed.). *CRC Handbook of Food Additives*. 2nd ed. Cleveland: The Chemical Rubber Co., 1972., p. 89

► [Hazardous Substances Data Bank \(HSDB\)](#)

The B vitamins are readily absorbed from the gastrointestinal tract, except in malabsorption syndromes. **Thiamine** is absorbed mainly in the duodenum.

USP Convention. *USPDI-Drug Information for the Health Care Professional*. 14th ed. Volume I. Rockville, MD: United States Pharmacopeial Convention, Inc., 1994. (Plus Updates)., p. 2647

► [Hazardous Substances Data Bank \(HSDB\)](#)

For more Absorption, Distribution and Excretion (Complete) data for **Vitamin B1** (8 total), please visit the [HSDB record page](#).

► [Hazardous Substances Data Bank \(HSDB\)](#)

9.4 Metabolism/Metabolites



Converted in vivo to **thiamine diphosphate**, a coenzyme in the decarboxylation of alpha-keto acids.

O'Neil, M.J. (ed.). *The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals*. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 1598

► [Hazardous Substances Data Bank \(HSDB\)](#)

Compound **3-(2'-methyl-4'-amino-5'-pyrimidylmethyl)-4-methylthiazole-5-acetic acid**, ie **thiamine acetic acid**, **2-methyl-4-amino-5-formylaminomethylpyrimidine**, and **5-(2-hydroxyethyl)-4-methylthiazole** have been identified as important metabolites of **thiamine**, **vitamin B1**.

The Chemical Society. *Foreign Compound Metabolism in Mammals. Volume 2: A Review of the Literature Published Between 1970 and 1971*. London: The Chemical Society, 1972., p. 248

► [Hazardous Substances Data Bank \(HSDB\)](#)

Biotransformation of **thiamine** in mammals is generally supposed to /yield/ **thiochrome**, **thiamine disulfide**, **5-(2-hydroxyethyl)-4-methyl-thiazole**, and some form corresponding to **pyrimidine** residue of **thiamine**.

The Chemical Society. *Foreign Compound Metabolism in Mammals. Volume 1: A Review of the Literature Published Between 1960 and 1969*. London: The Chemical Society, 1970., p. 229

► [Hazardous Substances Data Bank \(HSDB\)](#)

Thiamine is metabolized in the liver of animals. Several urinary metabolites of **thiamine** have been identified in humans. Little or no unchanged **thiamine** is excreted in urine following administration of physiologic doses; however, following administration of larger doses, both unchanged **thiamine** and metabolites are excreted after tissue stores become saturated.

American Society of Health System Pharmacists; *AHFS Drug Information 2009*. Bethesda, MD. (2009)

► [Hazardous Substances Data Bank \(HSDB\)](#)

9.5 Biological Half-Life



The biological half-life of the vitamin is in the range of 9-18 days.

Otten JJ, Hellwig JP, Meyers LD, eds; *Dietary Reference Intakes: The Essential Guide to Nutrient Requirements*, Washington, DC: The National Academies Press, 2006, p.281

► [Hazardous Substances Data Bank \(HSDB\)](#)

With higher pharmacological levels, namely repetitive 250-mg amounts taken orally and 500 mg given intramuscularly, nearly 1 week was required for steady state plasma concentrations to be reached; a mean elimination half-life of 1.8 days was estimated.

NAS, Food and Nutrition Board, Institute of Medicine; Dietary Reference Intakes for Thiamin, Riboflavin, Niacin, Vitamin B6, Folate, Vitamin B12, Pantothenic Acid, Biotin, and Choline. National Academy Press, Washington, D.C., pg. 59, 1998. Available from, as of March 2, 2010: <https://www.nap.edu/catalog/6015.html>

► [Hazardous Substances Data Bank \(HSDB\)](#)

Total **thiamin** content of the adult human has been estimated to be approximately 30 mg, and the biological half-life of the vitamin is probably in the range of 9 to 18 days.

NAS, Food and Nutrition Board, Institute of Medicine; Dietary Reference Intakes for Thiamin, Riboflavin, Niacin, Vitamin B6, Folate, Vitamin B12, Pantothenic Acid, Biotin, and Choline. National Academy Press, Washington, D.C., pg. 59, 1998. Available from, as of March 2, 2010: <https://www.nap.edu/catalog/6015.html>

► [Hazardous Substances Data Bank \(HSDB\)](#)

9.6 Mechanism of Action



Metabolic control analysis predicts that stimulators of transketolase enzyme synthesis such as **thiamin (vitamin B-1)** support a high rate of nucleic acid **ribose** synthesis necessary for tumor cell survival, chemotherapy resistance, and proliferation. Metabolic control analysis also predicts that transketolase inhibitor drugs will have the opposite effect on tumor cells. This may have important implications in the nutrition and future treatment of patients with cancer.

[PMID:10890024](#)

Cascante M et al; Nutr Cancer 36 (2): 150-4 (2000).

► [Hazardous Substances Data Bank \(HSDB\)](#)

10 Use and Manufacturing

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10.1 Uses

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EPA CPDat Chemical and Product Categories

The Chemical and Products Database, a resource for exposure-relevant data on chemicals in consumer products, Scientific Data, volume 5, Article number: 180125 (2018), DOI:10.1038/sdata.2018.125

▶ [EPA Chemical and Products Database \(CPDat\)](#)

Sources/Uses

Used as a human and veterinary vitamin (enzyme cofactor); [Merck Index] An important compound functioning as a component of the coenzyme [NAD](#). Its primary significance is in the prevention and/or cure of blacktongue and PELLAGRA. Most animals cannot manufacture this compound in amounts sufficient to prevent nutritional deficiency and it therefore must be supplemented through dietary intake. [ChemIDplus] Used as a flavoring agent and nutritional supplement for foods; [FDA] Permitted for use as an inert ingredient in non-food pesticide products; [EPA]

Merck Index - O'Neil MJ, Heckelman PE, Dobbelaar PH, Roman KJ (eds). The Merck Index, An Encyclopedia of Chemicals, Drugs, and Biologicals, 15th Ed. Cambridge, UK: The Royal Society of Chemistry, 2013.

▶ [Haz-Map, Information on Hazardous Chemicals and Occupational Diseases](#)

Prevention and treatment of [vitamin B1](#) deficiency

SRI

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

Medicine, nutrition, enriched flours. Isolated usually as the [chloride](#) ... Available as thiamine hydrochloride and [thiamine mononitrate](#)

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 1234

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

Reported uses

Table: Reported uses (ppm): (Flavor and Extract Manufacturers' Association)

Food Category	Usual	Max
Breakfast cereals	50.00	50.00
Condiments, relishes	50.00	50.00
Milk products	50.00	50.00
Nonalcoholic beverages	50.00	50.00

Burdock, G.A. (ed.). Fenaroli's Handbook of Flavor Ingredients. 6th ed.Boca Raton, FL 2010, p. 2014

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

THERAPEUTIC CATEGORY: Vitamin (enzyme cofactor)

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 1598

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

For more Uses (Complete) data for [Vitamin B1](#) (6 total), please visit the [HSDB record page](#).

10.1.1 Use Classification

Food additives -> Flavoring Agents

Human Drugs -> FDA Approved Drug Products with Therapeutic Equivalence Evaluations (Orange Book) -> Active Ingredients

Flavouring Agent -> FLAVOURING_AGENT; -> JECFA Functional Classes

Flavoring Agents -> JECFA Flavorings Index

Cosmetics -> Skin conditioning

513 | EUCOSMETICS | Combined Inventory of Ingredients Employed in Cosmetic Products (2000) and Revised Inventory (2006) | DOI:10.5281/zenodo.2624118

10.1.2 Industry Uses

Not Known or Reasonably Ascertainable

<https://www.epa.gov/chemical-data-reporting>

10.1.3 Consumer Uses

Not Known or Reasonably Ascertainable

<https://www.epa.gov/chemical-data-reporting>

10.1.4 Household Products

Household & Commercial/Institutional Products

Information on 5 consumer products that contain Thiamine hydrochloride in the following categories is provided:

- Landscaping/Yard
- Personal Care

10.2 Methods of Manufacturing

... /A method for the chemical synthesis of **thiamine**/ constructs the **thiazole** ring on a preformed **pyrimidine** intermediate. **Thiamine** manufacturers generally follow this approach. Some use **malonitrile** as the starting material for construction of the **4-amino-5-aminomethyl-2-methylpyrimidine** ring (also called **Grewe diamine**). Others start with **acrylonitrile** but all proceed via the key **Grewe diamine** intermediate through to thiothiamine.

Eggersdorfer M et al: Ullmann's Encyclopedia of Industrial Chemistry 7th ed. (2008). New York, NY: John Wiley & Sons; Vitamins. Online Posting Date: June 15, 2000

... /A method for the chemical synthesis of **thiamine** consists of separate syntheses of 4-amino-5-bromomethyl-2-methylpyrimidine hydrobromide and of the **thiazole** moiety or its **acetate**. Condensation of the two intermediate heterocycles gives **thiamine bromide hydrobromide** which is converted to thiamine chloride hydrochloride by treatment with **silver chloride** in **methanol** or with an ion-exchange resin.

Eggersdorfer M et al: Ullmann's Encyclopedia of Industrial Chemistry 7th ed. (2008). New York, NY: John Wiley & Sons; Vitamins. Online Posting Date: June 15, 2000

Reaction of **5-(beta-hydroxyethyl)-4-methylthiazole** with 2-methyl-4-amino-5-bromomethylpyrimidine, hydrogen bromide salt, followed by neutralization and reaction with **hydrochloric acid**

SRI

Hazardous Substances Data Bank (HSDB)

10.3 Impurities



Heavy metals: not more than 10 mg/kg; **water**: not more than 5%.

Burdock, G.A. (ed.). *Fennell's Handbook of Flavor Ingredients*. 4th ed.Boca Raton, FL 2002, p. 1790

Hazardous Substances Data Bank (HSDB)

10.4 Formulations/Preparations



Bulk Powder, Oral: Tablets: 25 mg, 50 mg, 100 mg, 250 mg, 500 mg. Parenteral Injection: 100 mg/mL. NOTE: Available from one or more manufacturer, distributor, and/or repackager by generic (nonproprietary) name.

American Society of Health System Pharmacists; AHFS Drug Information 2009. Bethesda, MD. (2009)

Hazardous Substances Data Bank (HSDB)

10.5 Consumption Patterns



100% in prevention and treatment of **vitamin B1** deficiency (1975)

SRI

Hazardous Substances Data Bank (HSDB)

10.6 U.S. Production



Aggregated Product Volume

2017: 13,228 lb

<https://www.epa.gov/chemical-data-reporting>

EPA Chemicals under the TSCA

(1972) Probably > 4.54 x 10+5 grams

SRI

Hazardous Substances Data Bank (HSDB)

(1975) Probably > 4.54 x 10+5 grams

SRI

Hazardous Substances Data Bank (HSDB)

(1986) No data

SRI

Hazardous Substances Data Bank (HSDB)

10.7 U.S. Imports



(1972) 1.09 X 10+8 g

SRI

Hazardous Substances Data Bank (HSDB)

(1975) 1.60 X 10+8 g (**Vitamin B1**)

SRI

Hazardous Substances Data Bank (HSDB)

(1984) 2.80X10+8 g **/Vitamin B1**, Thiamine hydrochloride or **Thiamine Mononitrate**, synthetic/

<https://pubchem.ncbi.nlm.nih.gov/compound/Thiamine-hydrochloride>

Bureau Of The Census. U.S. Imports For Consumption And General Imports 1984 p.1-368

► [Hazardous Substances Data Bank \(HSDB\)](#)

10.8 U.S. Exports



(1972) 1.34 X 10+7 g

SRI

► [Hazardous Substances Data Bank \(HSDB\)](#)

(1975) 5.78 X 10+6 g

SRI

► [Hazardous Substances Data Bank \(HSDB\)](#)

(1984) 3.36 X 10+7 g

Bureau Of The Census. U.S. Exports, Schedule E, 1984 p.2-100

► [Hazardous Substances Data Bank \(HSDB\)](#)

10.9 General Manufacturing Information



Industry Processing Sectors

Not Known or Reasonably Ascertainable

► [EPA Chemicals under the TSCA](#)

EPA TSCA Commercial Activity Status

Thiazolium, 3-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-5-(2-hydroxyethyl)-4-methyl-, **chloride**, hydrochloride (1:1:1): ACTIVE

<https://www.epa.gov/tsc-a-inventory>

► [EPA Chemicals under the TSCA](#)

Most of the **thiamine** commercially available is synthetic

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 1234

► [Hazardous Substances Data Bank \(HSDB\)](#)

Biosynthesized by microorganisms and plants. Dietary sources include whole grains, meat products, vegetables, milk, legumes and fruit. Also present in rice husks and yeast.

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 1598

► [Hazardous Substances Data Bank \(HSDB\)](#)

11 Identification



11.1 Analytic Laboratory Methods



AOAC Method 986.27- Fluorometric Method. The **thiamine** content of the sample is estimated by oxidizing **thiamine** to **thiochrome** and measuring fluorescence. Intensity of fluorescence is proportional to **thiamine** concentration.

Association of Official Analytical Chemists. Official Methods of Analysis. 15th ed. and Supplements. Washington, DC: Association of Analytical Chemists, 1990, p. 1113

► [Hazardous Substances Data Bank \(HSDB\)](#)

AOAC Method 953.17- **Thiamine** in Grain Products and Method 957.17-Thiamine in Bread. **Thiamine** is oxidized to **thiochrome** and the fluorescence measured.

Association of Official Analytical Chemists. Official Methods of Analysis. 15th ed. and Supplements. Washington, DC: Association of Analytical Chemists, 1990, p. 1051

► [Hazardous Substances Data Bank \(HSDB\)](#)

THE SPECIFIC **THIOCHROME** FLUORESCENCE ASSAY FOR **THIAMINE** WAS MODIFIED TO HANDLE MICROSAMPLES & TO USE 35S-**THIAMINE** LIQ SCINTILLATION ASSAY.

PMID:660465

PIPKIN JD ET AL; J PHARM SCI 67 (6): 818-821 (1978)

► [Hazardous Substances Data Bank \(HSDB\)](#)

HIGH-PRESSURE LIQ CHROMATOGRAPHY PROCEDURE FOR SIMULTANEOUS DETERMINATION OF **THIAMINE** WAS DEVELOPED & APPLIED TO ANALYSIS OF MULTIVITAMIN BLENDS.

PMID:151736

KIRCHMEIER RL ET AL; J PHARM SCI 67 (10): 1444-1446 (1978)

► [Hazardous Substances Data Bank \(HSDB\)](#)

4,4'-DIMETHOXY-DIQUINONE, REACTED QUANTITATIVELY WITH **VITAMIN B1** THUS OFFERING A SIMPLE & RAPID METHOD FOR ITS DETERMINATION. ABSORPTION PEAK WAS @ 490 NM.

ELDAWY MA ET AL; EGYPT J PHARM SCI 17 (2): 113-122 (1978)

► [Hazardous Substances Data Bank \(HSDB\)](#)

11.2 Clinical Laboratory Methods



Thiamin status can be assessed by determining erythrocyte transketolase activity, by measuring the concentration of **thiamin** and its phosphorylated esters in blood or serum components using high-performance liquid chromatography, or by measuring urinary **thiamin** excretion under basal conditions or after **thiamin** loading.

NAS, Food and Nutrition Board, Institute of Medicine; Dietary Reference Intakes for Thiamin, Riboflavin, Niacin, Vitamin B6, Folate, Vitamin B12, Pantothenic Acid, Biotin, and Choline. National Academy Press, Washington, D.C., pg. 60, 1998. Available from, as of March 2, 2010: <https://www.nap.edu/catalog/6015.html>

► [Hazardous Substances Data Bank \(HSDB\)](#)

The urinary excretion of **thiamin** is the indicator that has been used most widely in metabolic studies of **thiamin** requirements. ... Erythrocyte transketolase activity has also been widely used and is generally regarded as the best functional test of **thiamin** status, but it has some limitations for deriving the EAR and should be evaluated along with other indicators. In this test, erythrocytes are lysed and the transketolase activity is measured before and after stimulation by the addition of **thiamin** pyrophosphate (TPP); the basal level and the stimulated value (typically expressed as a multiple of the basal level, termed the activity coefficient or TPP effect) are measured. ... Factors other than **thiamin** status, such as genetic defects, may influence the enzyme activity and thus the test results.

NAS, Food and Nutrition Board, Institute of Medicine; Dietary Reference Intakes for Thiamin, Riboflavin, Niacin, Vitamin B6, Folate, Vitamin B12, Pantothenic Acid, Biotin, and Choline. National Academy Press, Washington, D.C., pg. 60-61, 1998. Available from, as of March 2, 2010: <https://www.nap.edu/catalog/6015.html>

► [Hazardous Substances Data Bank \(HSDB\)](#)

12 Safety and Hazards



12.1 Hazards Identification



12.1.1 GHS Classification



GHS Hazard Statements

Not Classified

Reported as not meeting GHS hazard criteria by 247 of 265 companies (only ~ 6.8% companies provided GHS information). For more detailed information, please visit [ECHA C&L website](#).

► [European Chemicals Agency \(ECHA\)](#)

12.1.2 Hazards Summary



Forms a [hydrate](#) on absorbing [water](#) from atmospheric humidity; [Merck Index] Safe when used as a flavoring agent in food; [JECFA] A skin and strong eye irritant; [Alfa Aesar MSDS] See [Thiamine](#).

Merck Index - O'Neil MJ, Heckelman PE, Dobbelaar PH, Roman KJ (eds). The Merck Index, An Encyclopedia of Chemicals, Drugs, and Biologicals, 15th Ed. Cambridge, UK: The Royal Society of Chemistry, 2013.

► [Haz-Map, Information on Hazardous Chemicals and Occupational Diseases](#)

12.2 Accidental Release Measures



12.2.1 Disposal Methods



SRP: Criteria for land treatment or burial (sanitary landfill) disposal practices are subject to significant revision. Prior to implementing land disposal of waste residue (including waste sludge), consult with environmental regulatory agencies for guidance on acceptable disposal practices.

► [Hazardous Substances Data Bank \(HSDB\)](#)

12.3 Handling and Storage



12.3.1 Storage Conditions



The drug is not highly susceptible to atmospheric oxidation but should be protected from air and light. Thiamine hydrochloride tablets should be stored in tight, light-resistant containers at a temperature less than 40 degrees C, preferably between 15-30 degrees C. Thiamine hydrochloride injection should be protected from light and stored at a temperature less than 40 degrees C, preferably between 15-30 degrees C; freezing should be avoided.

American Society of Health System Pharmacists; AHFS Drug Information 2009. Bethesda, MD. (2009)

► [Hazardous Substances Data Bank \(HSDB\)](#)

12.4 Other Safety Information



12.4.1 Special Reports



NAS, Food and Nutrition Board, Institute of Medicine; Dietary Reference Intakes for [Thiamin](#), [Riboflavin](#), [Niacin](#), [Vitamin B6](#), [Folate](#), [Vitamin B12](#), [Pantothenic Acid](#), [Biotin](#), and [Choline](#). National Academy Press, Washington, D.C. (1998).[Available from, as of March 2, 2010: <http://www.nap.edu/catalog/6015.html>]

► [Hazardous Substances Data Bank \(HSDB\)](#)

13 Toxicity



13.1 Toxicological Information



13.1.1 Acute Effects



► ChemIDplus

13.1.2 Interactions



... High dietary levels of thiamine hydrochloride have been reported to depress the metabolism of [zoxazolamine](#) and [aminopyrine](#) in rats without significantly altering the oxidative metabolism of hexobarbitone. /Thiamine hydrochloride/

The Chemical Society. Foreign Compound Metabolism in Mammals Volume 3. London: The Chemical Society, 1975., p. 594

► Hazardous Substances Data Bank (HSDB)

In rats treated with PCB, [vitamin B1](#) levels in blood, liver, and sciatic nerve decreased, transketolase activity decreased, and pyrophosphate effect increased. In DDT-treated rats, [vitamin B1](#) levels decreased in blood, brain, and liver, as did transketolase activity, while pyrophosphate effect increased.

PMID:109560

Yagi N et al; J Environ Pathol Toxicol 2 (4): 1119-1125 (1979).

► Hazardous Substances Data Bank (HSDB)

Although the clinical importance is unknown, [thiamine](#) reportedly may enhance the effect of neuromuscular blocking agents.

American Society of Health System Pharmacists; AHFS Drug Information 2009. Bethesda, MD. (2009)

► Hazardous Substances Data Bank (HSDB)

... Alcohol inhibits absorption of [thiamine](#).

USP Convention. USPDI-Drug Information for the Health Care Professional. 14th ed. Volume I. Rockville, MD: United States Pharmacopeial Convention, Inc., 1994. (Plus Updates)., p. 2647

► Hazardous Substances Data Bank (HSDB)

For more Interactions (Complete) data for [Vitamin B1](#) (9 total), please visit the [HSDB record page](#).

► Hazardous Substances Data Bank (HSDB)

13.1.3 Antidote and Emergency Treatment



/SRP:/ Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR if necessary. Immediately flush contaminated eyes with gently flowing [water](#). Do not induce vomiting. If vomiting occurs, lean patient forward or place on the left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. /Poisons A and B/

Currance, P.L. Clements, B., Bronstein, A.C. (Eds); Emergency Care For Hazardous Materials Exposure. 3Rd edition, Elsevier Mosby, St. Louis, MO 2005, p. 160

► Hazardous Substances Data Bank (HSDB)

/SRP:/ Basic treatment: Establish a patent airway (oropharyngeal or nasopharyngeal airway, if needed). Suction if necessary. Watch for signs of respiratory insufficiency and assist ventilations if needed. Administer [oxygen](#) by nonrebreather mask at 10 to 15 L/min. Monitor for pulmonary edema and treat if necessary Monitor for shock and treat if necessary Anticipate seizures and treat if necessary For eye contamination, flush eyes immediately with [water](#). Irrigate each eye continuously with 0.9% saline (NS) during transport Do not use emetics. For ingestion, rinse mouth and administer 5 mL/kg up to 200 mL of [water](#) for dilution if the patient can swallow, has a strong gag reflex, and does not drool Cover skin burns with dry sterile dressings after decontamination
/Poisons A and B/

Currance, P.L. Clements, B., Bronstein, A.C. (Eds.); *Emergency Care For Hazardous Materials Exposure*. 3Rd edition, Elsevier Mosby, St. Louis, MO 2005, p. 160

► [Hazardous Substances Data Bank \(HSDB\)](#)

/SRP:/ Advanced treatment: Consider orotracheal or nasotracheal intubation for airway control in the patient who is unconscious, has severe pulmonary edema, or is in severe respiratory distress. Positive-pressure ventilation techniques with a bag valve mask device may be beneficial. Consider drug therapy for pulmonary edema Consider administering a beta agonist such as [albuterol](#) for severe bronchospasm Monitor cardiac rhythm and treat arrhythmias as necessary Start IV administration of D5W /SRP: "To keep open", minimal flow rate/. Use 0.9% saline (NS) or lactated Ringer's if signs of hypovolemia are present. For hypotension with signs of hypovolemia, administer fluid cautiously. Watch for signs of fluid overload Treat seizures with [diazepam](#) or [lorazepam](#) Use [proparacaine hydrochloride](#) to assist eye irrigation /Poisons A and B/

Currance, P.L. Clements, B., Bronstein, A.C. (Eds.); *Emergency Care For Hazardous Materials Exposure*. 3Rd edition, Elsevier Mosby, St. Louis, MO 2005, p. 160-1

► [Hazardous Substances Data Bank \(HSDB\)](#)

13.1.4 Human Toxicity Excerpts



/SIGNS AND SYMPTOMS/ Adverse reactions with [thiamine](#) are rare, but hypersensitivity reactions have occurred, mainly after parenteral doses. These reactions have ranged in severity from very mild to, very rarely, fatal anaphylactic shock ... The UK Committee on Safety of Medicines had received, between 1970 and July, 1988, 90 reports of adverse reactions associated with the use of an injection containing high doses of vitamins B and C. The most frequent reactions were anaphylaxis (41 cases, including 2 fatalities), dyspnea or bronchospasm (13 cases), and rash or flushing (22 cases); 78 of the reactions occurred during, or shortly after, intravenous injection and the other 12 after intramuscular injection.

Sweetman SC (ed), Martindale: *The Complete Drug Reference*. London: Pharmaceutical Press (2009), p. 1976.

► [Hazardous Substances Data Bank \(HSDB\)](#)

/SIGNS AND SYMPTOMS/ Serious hypersensitivity/anaphylactic reactions can occur, especially after repeated administration. Deaths have resulted from IV or IM administration of [thiamine](#).

Novak, K.M. (ed.). *Drug Facts and Comparisons* 2008 Edition. Wolters Kluwer Health. St. Louis, Missouri 2008., p. 18

► [Hazardous Substances Data Bank \(HSDB\)](#)

/SIGNS AND SYMPTOMS/ Anaphylaxis. There have been occasional reports of serious and even fatal responses to the parenteral administration of [thiamin](#). The clinical characteristics have strongly suggested an anaphylactic reaction. Symptoms associated with [thiamin](#)-induced anaphylaxis include anxiety, pruritus, respiratory distress, nausea, abdominal pain, and shock, sometimes progressing to death.

NAS, Food and Nutrition Board, Institute of Medicine; *Dietary Reference Intakes for Thiamin, Riboflavin, Niacin, Vitamin B6, Folate, Vitamin B12, Pantothenic Acid, Biotin, and Choline*. National Academy Press, Washington, D.C., pg. 81, 1998. Available from, as of March 2, 2010: <https://www.nap.edu/catalog/6015.html>

► [Hazardous Substances Data Bank \(HSDB\)](#)

/SIGNS AND SYMPTOMS/ Allergic Sensitivity and Pruritus. One case of pruritus after an intake of 500 mg/day of [thiamin](#) intramuscularly /was reported/. Another study, which involved intravenous administration of 100 mg of [thiamin](#) hydrochloride to 989 patients, reported a burning effect at the injection site in 11 patients and pruritus in 1 patient. No reports of pruritus after [thiamin](#) ingestion were found.

NAS, Food and Nutrition Board, Institute of Medicine; *Dietary Reference Intakes for Thiamin, Riboflavin, Niacin, Vitamin B6, Folate, Vitamin B12, Pantothenic Acid, Biotin, and Choline*. National Academy Press, Washington, D.C., pg. 81, 1998. Available from, as of March 2, 2010: <https://www.nap.edu/catalog/6015.html>

► [Hazardous Substances Data Bank \(HSDB\)](#)

For more Human Toxicity Excerpts (Complete) data for [Vitamin B1](#) (13 total), please visit the [HSDB record page](#).

► [Hazardous Substances Data Bank \(HSDB\)](#)

13.1.5 Non-Human Toxicity Excerpts



/LABORATORY ANIMALS: Acute Exposure/ After iv injection of a high dose in cats, the cardiovascular system exhibited a 3 phase reaction. During phase 1, there was depression of heart rate and blood pressure, representing alpha-blockade, phase 2 reveals compensatory reflex mechanism, and 3 shows ganglionic blockade.

[PMID:74722](#)

Freye E et al; *Biomedicine* 28 (6): 315-319 (1978).

► [Hazardous Substances Data Bank \(HSDB\)](#)

/VETERINARY CASE REPORTS/ In sheep **thiamine tetrahydrofurfuryl disulfide** was im injected at a level of 50 mg/day. The injection appeared to increase urine and fecal **magnesium** excretion and decrease **magnesium tetrahydrofurfuryl disulfide**/

PMID:611158
Yano H, Kawashima R. J Nutr Sci Vitaminol 23 (6): 491-6 (1977).

► Hazardous Substances Data Bank (HSDB)

/OTHER TOXICITY INFORMATION/ **Thiamine** can give rise to toxic symptoms when administered parenterally. Mechanism of toxicity has been generally attributed to anaphylaxis, but may be due to ganglionic blocking.

► Hazardous Substances Data Bank (HSDB)

Clarke, E.G., and M. L. Clarke. *Veterinary Toxicology*. Baltimore, Maryland: The Williams and Wilkins Company, 1975., p. 176

13.1.6 Non-Human Toxicity Values



LD50 Rat sc 560 mg/kg

► Hazardous Substances Data Bank (HSDB)

Lewis, R.J. Sr. (ed) *Sax's Dangerous Properties of Industrial Materials*. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 3441

LD50 Rat iv 188 mg/kg

► Hazardous Substances Data Bank (HSDB)

Lewis, R.J. Sr. (ed) *Sax's Dangerous Properties of Industrial Materials*. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 3441

LD50 Mouse sc 301 mg/kg

► Hazardous Substances Data Bank (HSDB)

Lewis, R.J. Sr. (ed) *Sax's Dangerous Properties of Industrial Materials*. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 3441

LD50 Mouse iv 83 mg/kg

► Hazardous Substances Data Bank (HSDB)

Lewis, R.J. Sr. (ed) *Sax's Dangerous Properties of Industrial Materials*. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 3441

13.2 Ecological Information



13.2.1 Natural Pollution Sources



Vitamin B1 is found in all plants and animals; however, most organisms contain only low concentrations(1,2). It is found intracellularly in microorganisms, in plants (although unevenly distributed), and in tissue of animals, with the highest amounts occurring in the heart, kidney, liver, and brain(1). In plants, **vitamin B1** occurs predominantly as free **thiamine** and in animals it occurs almost entirely in phosphorylated forms, mainly **thiamine pyrophosphate**(2). It is biosynthesized by microorganisms and plants. Dietary sources include whole grains, meat products, vegetables, milk, legumes and fruit. **Vitamin B1** is also present in rice husks and yeast(3).

(1) Burdick D. Kirk-Othmer Encyclopedia of Chemical Technology. (2001). New York, NY: John Wiley & Sons: *Thiamine* (B1). Online Posting Date: Dec 4, 2000. (2) WHO: *Thiamin Deficiency and its Prevention and Control in Major Emergencies*. 1999. World Health Organization. Available from, as of August 19, 2010: https://whqlibdoc.who.int/hq/1999/WHO_NHD_99.13.pdf (3) O'Neil MJ, ed. *The Merck Index*. 14th ed., Whitehouse Station, NJ: Merck and Co., Inc., p. 1598 (2006)

► Hazardous Substances Data Bank (HSDB)

13.2.2 Food Survey Values



Dietary Sources of **Vitamin B1**(1).

Food	Thiamine Content, ug/100g
Wheat germ	2050
Dried brewer's yeast	1820
Soybean	1300
Pork	600-950
Dried beans and whey	500
Nuts	300-560
Brown rice	300
Beef liver	300

Food	Thiamine Content, ug/100g
Potatoes	170
Fish	50-90
Eggs	70
Vegetables (fruit, leaf, stem, root)	60-70
Whole milk	30-70
White rice	50

(1) Burdick D. Kirk-Othmer Encyclopedia of Chemical Technology. (2001). New York, NY: John Wiley & Sons. Thaimine (B1). Online Posting Date: Dec 4, 2000.

► Hazardous Substances Data Bank (HSDB)

Whole grain cereals, legumes such as beans and lentils, nuts, lean pork and yeast are rich sources of **vitamin B1**(1).

Food	Serving	Vitamin B1 (mg)
Lentils (cooked)	1/2 cup	0.17
Peas (cooked)	1/2 cup	0.21
Long grain brown rice (cooked)	1 cup	0.19
Long grain white rice, enriched (cooked)	1 cup	0.26
Long grain white rice unenriched (cooked)	1 cup	0.04
Whole wheat bread	1 slice	0.10
White bread, enriched	1 slice	0.11
Fortified breakfast cereal	1 cup	0.5-2.0
Wheat germ breakfast cereal	1 cup	4.47
Pork, lean (cooked)	3 ounces	0.72
Brazil nuts	1 ounce	0.18
Pecans	1 ounce	0.19
Spinach (cooked)	1/2 cup	0.09
Orange	1 fruit	0.10
Cantaloupe	1/2 fruit	0.11
Milk	1 cup	0.10
Egg (cooked)	1 large	0.03

(1) Linus Pauling Institute; Micronutrient Information Center. Thaimin. Oregon State University. Available from, as of August 20, 2010: <https://lpi.oregonstate.edu/info/center/vitamins/thiamin/index.html>

► Hazardous Substances Data Bank (HSDB)

13.2.3 Plant Concentrations



Natural sources of **vitamin B1** include whole cereal grains althouth processing of grains greatly reduces their **thiamin** content(1)/

(1) Cornell University; Plants Poisonous to Livestock. Toxic Agents in Plants. Thiaminases. Ithaca, NY: Cornell Univ., Dept Animal Sct. Available from, as of August 20, 2010: <https://www.ansci.cornell.edu/plants/toxicagents/index.html>

► Hazardous Substances Data Bank (HSDB)

13.2.4 Milk Concentrations



Vitamin B1 concentration range of 18.2 to 212.1 ug/L was reported in breast milk samples from Manila in a 1962 study of apparently healthy mothers. In another study, the mean **vitamin B1** content of breast milk in women from India, Thailand, and the US was 153, 93-149, and 142 ug/L, respectively(1).

(1) WHO. Thiamin Deficiency and its Prevention and Control in Major Emergencies. 1999. World Health Organization. Available from, as of August 19, 2010: https://whqlibdoc.who.int/hq/1999/WHO_NHD_99.13.pdf

► Hazardous Substances Data Bank (HSDB)

13.2.5 Probable Routes of Human Exposure



NIOSH (NOES Survey 1981-1983) has statistically estimated that 18,939 workers (9,502 of these were female) were potentially exposed to **vitamin B1** in the US(1).
(1) NIOSH; NOES. National Occupational Exposure Survey conducted from 1981-1983. Estimated numbers of employees potentially exposed to specific agents by 2-digit standard industrial classification (SIC). Available from, as of Feb 16, 2010: <https://www.cdc.gov/noes/>

► Hazardous Substances Data Bank (HSDB)

13.2.6 Average Daily Intake



In the US, the average dietary intake for **thiamine** for young adult men is about 2 mg/day and for young women, approximately 1.2 mg/day; over age 60, the average daily intake is about 1.4 and 1.1 mg/day for men and women, respectively(1).

(1) Linus Pauling Institute; Micronutrient Information Center. Thaimin. Oregon State University. Available from, as of August 20, 2010: <https://lpi.oregonstate.edu/info/center/vitamins/thiamin/index.html>

► Hazardous Substances Data Bank (HSDB)

13.2.7 Body Burden



Vitamin B1 concentration in a typical healthy human body is approximately 30 mg of **vitamine B1** in all forms with about 40-50% of this being in the muscles. Normal human blood contains about 90 ng/mL(1).

(1) Burdick D.; Kirk-Othmer Encyclopedia of Chemical Technology. (2001). New York, NY: John Wiley & Sons; Thaimine (B1). Online Posting Date: Dec 4, 2000.

► Hazardous Substances Data Bank (HSDB)

Vitamin B1 occurs in the human body as free **thiamine** and as **thiamine monophosphate**, **thiamine triphosphate**, and **thiamine pyrophosphate**. Beriberi is the disease resulting from severe **thiamine** deficiency; inadequate consumption of **thiamine** is the main cause of **thiamine** deficiency in underdeveloped countries. Alcoholism is the primary cause of **thiamine** deficiency in industrialized countries. Conditions resulting in an increased need for **thiamine** include strenuous physical exertion, fever, pregnancy, breast-feeding, and adolescent growth. Certain plants contain anti-thiamine factors which react with **thiamine** to form an oxidized, inactive product. Consuming large amounts of tea and coffee (including decaffeinated) have been associated with **thiamine** depletion in humans. Habitual consumption of raw freshwater fish, raw shellfish and ferns increase the risk of **thiamine** deficiency(1).

(1) Linus Pauling Institute; Micronutrient Information Center. Thaimin. Oregon State University. Available from, as of August 20, 2010: <https://lpi.oregonstate.edu/info/center/vitamins/thiamin/index.html>

► Hazardous Substances Data Bank (HSDB)

14 Associated Disorders and Diseases



► [Therapeutic Target Database \(TTD\)](#)

15 Literature

15.1 Coronavirus Studies

► PubChem

15.2 NLM Curated PubMed Citations

► PubChem

15.3 Springer Nature References

Springer Nature

15.4 Depositor Provided PubMed Citations



PubChem

15.5 Chemical Co-Occurrences in Literature



PubChem

15.6 Chemical-Gene Co-Occurrences in Literature





15.7 Chemical-Disease Co-Occurrences in Literature

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16 Patents



16.1 Depositor-Supplied Patent Identifiers



► PubChem

[Link to all deposited patent identifiers](#)

► PubChem

16.2 WIPO PATENTSCOPE



Patents are available for this chemical structure:

<https://patentscope.wipo.int/search/en/result.jsf?inchikey=DPJRMOMPQZCRJU-UHFFFAOYSA-M>

► PATENTSCOPE (WIPO)

17 Interactions and Pathways



17.1 Chemical-Target Interactions



◀ ChEMBL

19 Classification



19.1 MeSH Tree



► Medical Subject Headings (MeSH)

19.2 NCI Thesaurus Tree



► NCI Thesaurus (NCIt)

19.3 ChEBI Ontology



◀ CHEBI

19.4 KEGG: Drug



◀ KEGG

19.5 KEGG: ATC



◀ KEGG

19.6 KEGG: JP15



◀ KEGG

19.7 KEGG: OTC drugs



◀ KEGG

19.8 ChemDplus



◀ ChemDplus

19.9 ChEMBL Target Tree



► CHEMBL

19.10 UN GHS Classification



► UN Globally Harmonized System of Classification and Labelling of Chemicals (GHS)

19.11 EPA CPDat Classification



► EPA Chemical and Products Database (CPDat)

19.12 NORMAN Suspect List Exchange Classification



▶ NORMAN Suspect List Exchange

19.13 EPA DSSTox Classification



▶ EPA DSSTox

19.14 Consumer Product Information Database Classification



▶ Consumer Product Information Database (CPID)

19.15 FDA Drug Type and Pharmacologic Classification





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Thiamine hydrochloride

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Thiamine hydrochloride

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THIAMINE HYDROCHLORIDE

<https://gsrs.ncats.nih.gov/ginas/app/beta/substances/M572600ESP>

8. Hazardous Substances Data Bank (HSDB)

Vitamin B1

<https://pubchem.ncbi.nlm.nih.gov/source/hsdb/220>

9. ChEBI

Thiamine hydrochloride

<http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:49105>

ChEBI Ontology

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Thiamine hydrochloride

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Thiamine hydrochloride

<https://www.fao.org/food/food-safety-quality/scientific-advice/jecfa/jecfa-flav/details/en/c/963/>

THIAMINE HYDROCHLORIDE

<https://apps.who.int/food-additives-contaminants-jecfa-database/Home/Chemical/4242>

VITAMIN B1 HYDROCHLORIDE

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<https://www.fda.gov/about-fda/about-website/website-policies#linking>

THIAMINE HYDROCHLORIDE

<https://www.cfsanappsexternal.fda.gov/scripts/fdcc/index.cfm?set=FoodSubstances&id=THIAMINEHYDROCHLORIDE>

23. Flavor and Extract Manufacturers Association (FEMA)

THIAMINE HYDROCHLORIDE

<https://www.femaflavor.org/flavor-library/thiamine-hydrochloride>

24. Human Metabolome Database (HMDB)

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<http://www.hmdb.ca/citing>

HMDB0303167_nmr_one_3958

<https://hmdb.ca/metabolites/HMDB0303167#spectra>

25. SpectraBase

THIAMINE, MONOHYDROCHLORIDE

<https://spectrabase.com/spectrum/GaICEPUMGfQ>

THIAMINE, HYDROCHLORIDE

<https://spectrabase.com/spectrum/4YC1ujPjy0v>

THIAMIN, HYDROCHLORIDE

<https://spectrabase.com/spectrum/4eD5ZyVYXbX>

Thiamine HCl (Vitamin B1)

<https://spectrabase.com/spectrum/7wj1qjU7aYl>

thiamine hydrochloride

<https://spectrabase.com/spectrum/HFkTU1PFd2o>

3-((4-amino-2-methylpyrimidin-5-yl)methyl)-5-(2-hydroxyethyl)-4-methylthiazol-3-ium chloride hydrochloride

<https://spectrabase.com/spectrum/8e34mNwybaK>

26. National Drug Code (NDC) Directory

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THIAMINE HCL

<https://www.fda.gov/drugs/drug-approvals-and-databases/national-drug-code-directory>

27. NLM RxNorm Terminology

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<https://www.nlm.nih.gov/research/umls/rxnorm/docs/termsofservice.html>

thiamine hydrochloride
<https://rxnav.nlm.nih.gov/id/rxnorm/235355>

28. PubChem

<https://pubchem.ncbi.nlm.nih.gov>

29. Springer Nature

<https://pubchem.ncbi.nlm.nih.gov/substance/?source=15745&sourceid=20051189-789530474>

30. Therapeutic Target Database (TTD)

Thiamine Hydrochloride
<http://idrblab.net/ttd/data/drug/details/D02LDV>

31. Wikidata

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thiamine hydrochloride
<https://www.wikidata.org/wiki/Q27121486>

32. Wikipedia

thiamine hydrochloride
https://en.wikipedia.org/wiki/Thiamine_hydrochloride

33. Medical Subject Headings (MeSH)

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thiamine hydrochloride
<https://www.ncbi.nlm.nih.gov/mesh/2099392>

MeSH Tree
<http://www.nlm.nih.gov/mesh/meshhome.html>

34. KEGG

LICENSE
Academic users may freely use the KEGG website. Non-academic use of KEGG generally requires a commercial license
<https://www.kegg.jp/kegg/legal.html>

Therapeutic category of drugs in Japan
http://www.genome.jp/kegg-bin/get_htext?br08301.keg

Anatomical Therapeutic Chemical (ATC) classification
http://www.genome.jp/kegg-bin/get_htext?br08303.keg

Drugs listed in the Japanese Pharmacopoeia
http://www.genome.jp/kegg-bin/get_htext?br08311.keg

Classification of Japanese OTC drugs
http://www.genome.jp/kegg-bin/get_htext?br08313.keg

35. UN Globally Harmonized System of Classification and Labelling of Chemicals (GHS)

GHS Classification Tree
http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html

36. EPA Substance Registry Services

LICENSE
<https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources>

EPA SRS List Classification
https://sor.epa.gov/sor_internet/registry/substreg/LandingPage.do

37. PATENTSCOPE (WIPO)

SID 403035113
<https://pubchem.ncbi.nlm.nih.gov/substance/403035113>