

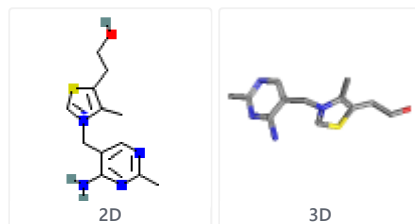
COMPOUND SUMMARY

Thiamine

PubChem CID

1130

Structure

[Find Similar Structures](#)

Molecular Formula

C₁₂H₁₇N₄OS⁺

Synonyms

thiamine
thiamin
vitamin B1
Aneurin
Thiamine ion[More...](#)

Molecular Weight

265.36

Dates

Modify	Create
2022-11-12	2004-09-16

Thiamine is a heat-labile and [water](#)-soluble essential vitamin, belonging to the vitamin B family, with antioxidant, erythropoietic, mood modulating, and [glucose](#)-regulating activities. Thiamine reacts with [adenosine triphosphate \(ATP\)](#) to form an active coenzyme, [thiamine pyrophosphate](#). [Thiamine pyrophosphate](#) is necessary for the actions of [pyruvate](#) dehydrogenase and [alpha-ketoglutarate](#) in carbohydrate metabolism and for the actions of transketolase, an enzyme that plays an important role in the pentose phosphate pathway. Thiamine plays a key role in intracellular [glucose](#) metabolism and may inhibit the action of [glucose](#) and insulin on arterial smooth muscle cell proliferation. Thiamine may also protect against lead toxicity by inhibiting lead-induced lipid peroxidation.

[► NCI Thesaurus \(NCIt\)](#)

Thiamine or thiamin, also known as **vitamin B1**, is a colorless compound with the chemical formula C₁₂H₁₇N₄O₅. It is soluble in **water** and insoluble in alcohol. Thiamine decomposes if heated. Thiamine was first discovered by Umetaro Suzuki in Japan when researching how rice bran cured patients of Beriberi. Thiamine plays a key role in intracellular **glucose** metabolism and it is thought that thiamine inhibits the effect of **glucose** and insulin on arterial smooth muscle cell proliferation. Thiamine plays an important role in helping the body convert carbohydrates and fat into energy. It is essential for normal growth and development and helps to maintain proper functioning of the heart and the nervous and digestive systems. Thiamine cannot be stored in the body; however, once absorbed, the vitamin is concentrated in muscle tissue.

► [DrugBank](#)

Thiamine(1+) is a primary alcohol that is **1,3-thiazol-3-ium** substituted by (4-amino-2-methylpyrimidin-5-yl)methyl, **methyl** and 2-hydroxyethyl groups at positions 3, 4 and 5, respectively. It has a role as a human metabolite, a *Saccharomyces cerevisiae* metabolite, an *Escherichia coli* metabolite and a mouse metabolite. It is a primary alcohol and a **vitamin B1**. It is a conjugate base of a thiamine(2+).

► [ChEBI](#)

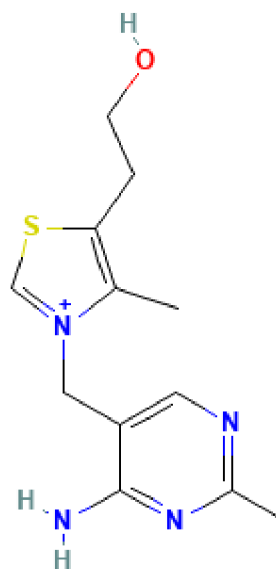
1 Structures



1.1 2D Structure



Chemical Structure
Depiction



► PubChem

1.2 3D Conformer



► 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

Computed by Lexichem TK 2.7.0 (PubChem release 2021.05.07)

► [PubChem](#)

2.1.2 InChI



InChI=1S/C12H17N4OS/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)/q+1

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

► [PubChem](#)

2.1.3 InChIKey



JZRWCGZRTZMZEH-UHFFFAOYSA-N

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

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

► [PubChem](#)

2.2 Molecular Formula



C12H17N4OS+

Computed by PubChem 2.1 (PubChem release 2021.05.07)

► [PubChem](#)

2.3 Other Identifiers



2.3.1 CAS



70-16-6

► CAS Common Chemistry; ChemIDplus; DrugBank; EPA DSSTox; FDA Global Substance Registration System (GSRS); Human Metabolome Database (HMDB)

59-43-8

► European Chemicals Agency (ECHA); Hazardous Substances Data Bank (HSDB)

2.3.2 European Community (EC) Number



200-425-3

► European Chemicals Agency (ECHA)

2.3.3 UNII



4ABT0J945J

► FDA Global Substance Registration System (GSRS)

2.3.4 DSSTox Substance ID



DTXSID50220251

► EPA DSSTox

2.3.5 Wikidata



Q83187

► Wikidata

2.3.6 NCI Thesaurus Code



C874

► NCI Thesaurus (NCIt)

2.3.7 RXCUI



1546268

► NLM RxNorm Terminology

2.4 Synonyms



2.4.1 MeSH Entry Terms



Aneurin
Mononitrate, Thiamine
Thiamin
Thiamine
Thiamine Mononitrate
Vitamin B 1
Vitamin B1

► Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms



thiamine	thiaminium	3-((4-Amino-2-methylpyrimidin-5-yl)methyl)-5-(2-hydroxyethyl
thiamin	thiamine(1+)	Thiazolium, 3-((4-amino-2-methyl-5-pyrimidinyl)methyl)-5-(2-l
vitamin B1	thiamine(1+) ion	[3H]thiamine
Aneurin	3-[(4-amino-2-methylpyrimidin-5-yl)methyl]-5-(2-hydroxyethyl)-4-methyl-1,3-thiazol-3-ium	[3H]-thiamine
Thiamine ion	2-[3-[(4-amino-2-methylpyrimidin-5-yl)methyl]-4-methyl-1,3-thiazol-3-ium-5-yl]ethanol	Vitamin B 1
Antiberiberi factor	Thiamine (Vit B1)	NSC36226
Thiadoxine	4ABT0J945J	[3H]vitamin B1
Betaxin	CHEBI:18385	1sbr
70-16-6	3-(4-AMINO-2-METHYL-PYRIMIDIN-5-YLMETHYL)-5-(2-HYDROXY-ETHYL)-4-METHYL-THIAZOL-3-IUM	3rlb
Biamine	VIB	ThOH
Bequin	THD	Prestwick0_000631

► PubChem

3 Chemical and Physical Properties

?

3.1 Computed Properties

?

Property Name	Property Value	Reference
Molecular Weight	265.36	Computed by PubChem 2.1 (PubChem release 2021.05.07)
XLogP3-AA	1	Computed by XLogP3 3.0 (PubChem release 2021.05.07)
Hydrogen Bond Donor Count	2	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Hydrogen Bond Acceptor Count	5	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	265.11230735	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Monoisotopic Mass	265.11230735	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	18	Computed by PubChem
Formal Charge	1	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	1	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2021.05.07)

► PubChem

3.2 Experimental Properties

?

3.2.1 Physical Description

?

Solid with a slight odor; [HSDB] Crystals; [Avocado Research MSDS]

► Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

Solid

► [Human Metabolome Database \(HMDB\)](#)

3.2.2 Color/Form



Crystals from water

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 \(HSDB\)](#)

3.2.3 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



248 dec °C

PhysProp

► [DrugBank](#)

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. Furia and N. Bellanca. 2nd ed. Cleveland: The Chemical Rubber Co., 1975., p. 562

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

248 °C

► [Human Metabolome Database \(HMDB\)](#)

3.2.5 Solubility



500000 mg/L

MERCK INDEX (1996); approx.

► [DrugBank](#)

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

Furia, 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 \(HSDB\)](#)

500.0 mg/mL

► [Human Metabolome Database \(HMDB\)](#)

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.html>

► [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)

Furia, 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/

Furia, 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

Furia, 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

Furia, 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 Collision Cross Section



162.4 Å² [M+H]⁺ [CCS Type: DT, Method: single field calibrated with Agilent tune mix (Agilent)]

<https://pubs.acs.org/doi/abs/10.1021/acs.analchem.6b03091>

► [CCSbase](#)

160.3 Å² [M-H]⁻ [CCS Type: DT, Method: single field calibrated with Agilent tune mix (Agilent)]

<https://pubs.acs.org/doi/abs/10.1021/acs.analchem.6b03091>

► [CCSbase](#)

159 Å² [M]⁺ [CCS Type: TW, Method: calibrated with [polyalanine](#)]

<https://pubs.acs.org/doi/abs/10.1021/ac500405x>

► [CCSbase](#)

162.8 Å² [M]⁺ [CCS Type: DT, Method: single field calibrated with ESI Low Concentration Tuning Mix (Agilent)]

<https://pubs.acs.org/doi/abs/10.1021/acs.analchem.8b04322>

► CCSbase

155.9 Å² [M+H]⁺ [CCS Type: TW, Method: calibrated with [polyalanine](#) and drug standards]

<https://pubs.acs.org/doi/abs/10.1021/acs.analchem.7b01709>

► CCSbase

163 Å² [M*]⁺

550 | CCSCOMPEND | *The Unified Collision Cross Section (CCS) Compendium* | [DOI:10.5281/zenodo.2658162](https://doi.org/10.5281/zenodo.2658162)

► NORMAN Suspect List Exchange

3.2.10 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 Rheinhold, 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 \(HSDB\)](#)

3.2.11 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



Showing 2 of 3 [View More](#)

Spectra ID	1255
Instrument Type	Varian
Frequency	500 MHz
Solvent	Water
pH	7.00
Shifts [ppm]:Intensity	2.52:87.66, 2.55:100.00, 3.16:14.44, 3.18:24.56, 3.19:12.02, 3.86:10.23, 3.87:13.24, 3.89:6.39, 5.47:59.70, 8.03:38.62, 9.47:2.21
Thumbnail	

▶ [Human Metabolome Database \(HMDB\)](#)

Spectra ID	4799
Instrument Type	Bruker
Solvent	D2O

pH	7.4
Shifts [ppm]:Intensity	2.49:380625.00, 2.58:368163.00, 3.18:57419.00, 3.19:107591.00, 3.21:60207.00, 3.88:68842.00, 3.89:120330.00, 3.90:61215.00, 5.46:210998.00, 8.06:124405.00
Thumbnail	

▶ [Human Metabolome Database \(HMDB\)](#)

4.1.2 13C NMR Spectra

?

↗

Showing 2 of 5 [View More](#) 

Spectra ID	1211
Instrument Type	Bruker
Frequency	125 MHz
Solvent	Water
pH	7.00
Shifts [ppm]:Intensity	0.00:4.14, 107.36:15.88, 13.73:32.95, 138.82:13.89, 145.48:14.98, 156.60:25.71, 159.61:42.30, 164.46:17.35, 171.61:19.02, 26.70:27.24, 31.87:39.30, 53.62:40.68, 63.12:44.96
Thumbnail	



► [Human Metabolome Database \(HMDB\)](#)

Spectra ID	166493
Frequency	400 MHz
Solvent	H2O
Shifts [ppm]	107.36, 13.73, 138.82, 145.48, 156.60, 159.61, 164.46, 171.61, 26.70, 31.87, 53.62, 63.12
Thumbnail	

► [Human Metabolome Database \(HMDB\)](#)

4.2 2D NMR Spectra

4.2.1 1H-1H NMR Spectra



2D NMR Spectra Type	1H-1H TOCSY
Spectra ID	1004
Shifts [ppm] (F2:F1)	2.37:2.49, 2.48:2.58, 2.50:2.50, 2.58:2.59, 3.20:3.20, 3.20:3.90, 3.90:3.20, 3.90:3.90, 4.82:4.82, 5.47:5.47, 8.09:8.07
Thumbnail	

▶ [Human Metabolome Database \(HMDB\)](#)

4.2.2 1H-13C NMR Spectra



2D NMR Spectra Type	1H-13C HSQC
Spectra ID	1228
Instrument Type	Bruker
Frequency	600 MHz
Solvent	Water
pH	7.00
Shifts [ppm] (F2:F1):Intensity	2.49:26.74:0.81, 2.57:13.78:0.07, 3.18:31.88:0.54, 3.89:63.21:0.58, 5.45:53.87:1.00, 8.05:159.72:0.03, 9.42:156.57:0.04
Thumbnail	



► [Human Metabolome Database \(HMDB\)](#)

4.3 Mass Spectrometry



4.3.1 GC-MS



Instrument Name	DI
Source of Spectrum	Chemical Concepts, A Wiley Division, Weinheim, Germany
Copyright	Copyright © 2002-2021 Wiley-VCH Verlag GmbH & Co. KGaA. All Rights Reserved.
Thumbnail	



► SpectraBase

Source of Spectrum	QA-33-176-0
Copyright	Copyright© 2020-2021;John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

► SpectraBase

4.3.2 MS-MS

?

Showing 2 of 6 View More

Spectra ID	2238527
Ionization Mode	Negative
SPLASH	splash10-0002-0940000000-561b322c315b79ac7e85
Top 5 Peaks	147.0685 100 233.0925 44.81 263.103 9.60 59.01401 1.55



► [Human Metabolome Database \(HMDB\)](#)

Spectra ID	2239039
Ionization Mode	Negative
SPLASH	splash10-0002-0900000000-5ef00213f89b8eaadfca
Top 5 Peaks	147.0685 100 120.0561 2.22 59.01401 1.88 132.0573 1.39 104.0287 1.36
Thumbnail	



► [Human Metabolome Database \(HMDB\)](#)

4.3.3 LC-MS



Showing 2 of 23 [View More](#)

Accession ID	MSBNK-Keio_Univ-KO001933
Authors	Kakazu Y, Horai H, Institute for Advanced Biosciences, Keio Univ.
Instrument	API3000, Applied Biosystems
Instrument Type	LC-ESI-QQ
MS Level	MS2
Ionization Mode	NEGATIVE
Collision Energy	10 V
Precursor m/z	263
Precursor Adduct	[M-2H]-
Top 5 Peaks	263.1 999 233.2 283 147.1 17 171 14 58.9 2
SPLASH	splash10-03di-0090000000-872150be83cbd75d8ecf
Thumbnail	

License	CC BY-NC-SA
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► [MassBank Europe](#)

Accession ID	MSBNK-Keio_Univ-KO001934
Authors	Kakazu Y, Horai H, Institute for Advanced Biosciences, Keio Univ.
Instrument	API3000, Applied Biosystems
Instrument Type	LC-ESI-QQ
MS Level	MS2
Ionization Mode	NEGATIVE
Collision Energy	20 V
Precursor m/z	263
Precursor Adduct	[M-2H]-
Top 5 Peaks	147.1 999 233.1 398 263.3 34 171.5 18 59.1 6
SPLASH	splash10-0002-0930000000-ecf71c75bdea859139d5

Thumbnail	
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License	CC BY-NC-SA
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► [MassBank Europe](#)

4.3.4 Other MS



Showing 2 of 5 [View More](#)

MoNA ID	CCMSLIB00000479740
MS Category	Experimental
MS Level	MS2
Precursor Type	[M+H] ⁺
Precursor m/z	266.114
Instrument	Orbitrap
Ionization Mode	positive
Top 5 Peaks	122.077019 100 144.055710 29.90 265.137939 6.68 81.047157 3.23 218.999146 0.87
SPLASH	splash10-00di-0900000000-c8cf7d3a7bd209262162
Thumbnail	

Submitter	GNPS Team, University of California, San Diego
-----------	--

► [MassBank of North America \(MoNA\)](#)

MoNA ID	PS035001
MS Category	Experimental
MS Level	MS2
Precursor m/z	265.31
Instrument	TQD, Waters
Instrument Type	Flow-injection QqQ/MS
Ionization	ESI
Ionization Mode	positive
Top 5 Peaks	265 100 122 28.66 144 7.58 264 4.50 121 3.47
SPLASH	splash10-014i-0390000000-93fbdda344c4a410fedf
Thumbnail	

Submitter	ReSpect Consortium, RIKEN Center for Sustainable Resource Science
-----------	---

▶ [MassBank of North America \(MoNA\)](#)

4.4 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/

Weast, R.C. (ed.). Handbook of Chemistry and Physics. 60th ed. Boca Raton, Florida: CRC Press Inc., 1979., p. C-543

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

4.5 IR Spectra

?

↗

4.5.1 FTIR Spectra

?

↗

Instrument Name	Bruker IFS 85
Technique	KBr-Pellet
Copyright	Copyright © 1989, 1990-2021 Wiley-VCH Verlag GmbH & Co. KGaA. 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 \(HSDB\)](#)

5 Related Records

5.1 Related Compounds with Annotation

► PubChem

5.2 Related Compounds

Same Connectivity	8 Records
Same Parent, Connectivity	134 Records
Same Parent, Exact	121 Records
Mixtures, Components, and Neutralized Forms	278 Records
Similar Compounds	297 Records
Similar Conformers	74 Records

► PubChem

5.3 Substances

5.3.1 Related Substances



All	1,076 Records
Same	133 Records
Mixture	943 Records

▶ PubChem

5.3.2 Substances by Category



▶ PubChem

5.4 Entrez Crosslinks



PubMed	3,894 Records
Protein Structures	12 Records
Taxonomy	4 Records
OMIM	1 Record
Gene	38 Records

[▶ PubChem](#)

5.5 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 \(HSDB\)](#)

5.6 NCBI LinkOut





6 Chemical Vendors



► PubChem

7 Drug and Medication Information



7.1 Drug Indication



For the treatment of thiamine and [niacin](#) deficiency states, Korsakov's alcoholic psychosis, Wernicke-Korsakov syndrome, delirium, and peripheral neuritis.

▶ [DrugBank](#)

7.2 WHO Essential Medicines



Drug	Drug Classes	Formulation	Indication
Thiamine	Vitamins and minerals	Oral - Solid: 50 mg (hydrochloride)	Vitamin B1 deficiency [co-prescribed with A11DA01]

▶ [WHO Model Lists of Essential Medicines](#)

7.3 FDA Orange Book



▶ [FDA Orange Book](#)

7.4 FDA National Drug Code Directory



THIAMINE is an active ingredient in 18 products including: 'B-BALANCE LIQUESCENCE', 'CELLULAR OXYGENATOR DROPS', and 'CITRANATAL 90 DHA'.

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

7.5 Drug Labels for Ingredients



Label Information	Total 7 labels
Drug Ingredient	ASCORBIC ACID; BIOTIN; CHOLECALCIFEROL; CYANOCOBALAMIN; DEXPANTHENOL; FOLIC ACID; NIACINAMIDE; PYRIDOXINE; RIBOFLAVIN; THIAMINE; TOCOPHEROL ACETATE; VITAMIN A; VITAMIN K
NDC Code(s)	54643-5646-0, 54643-5646-1, 54643-5647-0, 54643-5649-1, 54643-5650-2, 54643-7862-1, 54643-7874-2, 54643-7886-1, 54643-7898-0, 54643-9007-1, 54643-9015-2, 54643-9023-1, 54643-9031-0
Packagers	Sandoz Manufacturing Inc

▶ [DailyMed](#)

Label Information	Total 389 labels
Drug Ingredient	THIAMINE
NDC Code(s)	0178-0716-90, 0178-0821-30, 0178-0829-30, 0178-0858-90, 0178-0859-90, 0178-0864-30, 0178-0891-30, 0178-0893-30, 0178-0894-30, 0178-0898-30 ... total 341.
Packagers	7T Pharma LLC; A-S Medication Solutions; AMELLA PHARMA, LLC; ANUBIS COSMETICS SL; Acella Pharmaceuticals, LLC; Advanced Pharmaceutical Services, Inc. Dba Affordable Quality Pharmaceuticals; Agile RX; Agri Laboratories, Inc.; Agri Laboratories, Ltd.; Akron Pharma ... total 154.

▶ [DailyMed](#)

7.6 Clinical Trials



7.6.1 ClinicalTrials.gov



► [ClinicalTrials.gov](#)

7.6.2 EU Clinical Trials Register



► [EU Clinical Trials Register](#)

7.7 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 \(HSDB\)](#)

7.8 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 \(HSDB\)](#)

7.9 Biomarker Information



► MarkerDB

8 Food Additives and Ingredients



8.1 FDA Substances Added to Food



Substance	THIAMINE
Used for (Technical Effect)	NUTRIENT SUPPLEMENT

▶ [FDA Center for Food Safety and Applied Nutrition \(CFSAN\)](#)

9 Pharmacology and Biochemistry



9.1 Pharmacodynamics



Thiamine is a vitamin with antioxidant, erythropoietic, cognition-and mood-modulatory, antiatherosclerotic, putative ergogenic, and detoxification activities. Thiamine has been found to protect against lead-induced lipid peroxidation in rat liver and kidney. Thiamine deficiency results in selective neuronal death in animal models. The neuronal death is associated with increased free radical production, suggesting that oxidative stress may play an important early role in brain damage associated with thiamine deficiency. Thiamine plays a key role in intracellular [glucose](#) metabolism and it is thought that thiamine inhibits the effect of [glucose](#) and insulin on arterial smooth muscle cell proliferation. Inhibition of endothelial cell proliferation may also promote atherosclerosis. Endothelial cells in culture have been found to have a decreased proliferative rate and delayed migration in response to hyperglycemic conditions. Thiamine has been shown to inhibit this effect of [glucose](#) on endothelial cells.

► [DrugBank](#)

9.2 MeSH Pharmacological Classification



Vitamin B Complex

A group of water-soluble vitamins, some of which are COENZYMES. (See [all compounds classified as Vitamin B Complex](#).)

► [Medical Subject Headings \(MeSH\)](#)

9.3 ATC Code



A - Alimentary tract and metabolism

A11 - Vitamins

A11D - **Vitamin b1**, plain and in combination with **vitamin b6** and b12

A11DA - Vitamin b1, plain

A11DA01 - Thiamine (vit B1)

► [WHO Anatomical Therapeutic Chemical \(ATC\) Classification](#)

9.4 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	

Life Stage Group	Estimated Average Requirement	Recommended Dietary Allowance	Adequate Intake
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 \(HSDB\)](#)

9.5 Absorption, Distribution and Excretion



Absorption

Absorbed mainly from duodenum, by both active and passive processes

► [DrugBank](#)

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 \(HSDB\)](#)

9.6 Metabolism/Metabolites



Hepatic

► [DrugBank](#)

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 \(HSDB\)](#)

9.7 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 \(HSDB\)](#)

9.8 Mechanism of Action



It is thought that the mechanism of action of thiamine on endothelial cells is related to a reduction in intracellular protein glycation by redirecting the glycolytic flux. Thiamine is mainly the transport form of the vitamin, while the active forms are phosphorylated thiamine derivatives. Natural derivatives of [thiamine phosphate](#), such as [thiamine monophosphate \(ThMP\)](#), [thiamine diphosphate \(ThDP\)](#), also sometimes called [thiamine pyrophosphate \(TPP\)](#), [thiamine triphosphate \(ThTP\)](#), and [thiamine triphosphate \(AThTP\)](#), that act as coenzymes in addition to their each unique biological functions.

► [DrugBank](#)

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 \(HSDB\)](#)

9.9 Human Metabolite Information



9.9.1 Tissue Locations



Adipose Tissue
Adrenal Gland
Brain
Erythrocyte

Fibroblasts
Intestine
Kidney
Liver
Neuron
Placenta
Skeletal Muscle
Testis

► [Human Metabolome Database \(HMDB\)](#)

9.9.2 Cellular Locations



Extracellular
Membrane
Mitochondria

► [Human Metabolome Database \(HMDB\)](#)

9.9.3 Metabolite Pathways



Thiamine Metabolism

► [Human Metabolome Database \(HMDB\)](#)

9.10 Biochemical Reactions



► [Rhea - Annotated Reactions Database](#)

► [PubChem](#)

10 Use and Manufacturing

10.1 Uses

Sources/Uses

An essential vitamin for carbohydrate metabolism and nerve function; Found in whole grains, meats, vegetables, milk, legumes, fruit, rice husks, and yeast; [Merck Index] Used as a nutritional supplement and flavoring agent for foods; [FDA] Used as a medicine, nutrient, in enriched flours, and other foods; [HSDB]

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](#).

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

10.1.1 Use Classification



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

► [FDA Orange Book](#)

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

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

... /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

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

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.). Fenaroli'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



(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/

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



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 Hazards Summary



A [water](#)-soluble vitamin used to treat beriberi and Wernicke-Korsakoff syndrome; Anaphylactoid reactions were reported after intravenous injection--rare with new preparations; [Olson, p. 628] Hydrochloride: Safe when used as a flavoring agent in food; [JECFA] Occupational asthma confirmed with broncho-provocation testing in a worker manufacturing cereal; [Malo]

Olson - Olson KR (ed). Poisoning & Drug Overdose, 7th Ed. New York: Lange Medical Books/McGraw-Hill, 2018., p. 628

► [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 Toxicity Summary

?

Thiamine toxicity is uncommon; as excesses are readily excreted, although long-term supplementation of amounts larger than 3 gram have been known to cause toxicity. Oral mouse LD₅₀ = 8224 mg/kg, oral rat LD₅₀ = 3710 mg/kg.

▶ DrugBank

13.1.2 Drug Induced Liver Injury

?

Compound	thiamine
DILI Annotation	No-DILI-Concern
Label Section	No match
References	M Chen, V Vijay, Q Shi, Z Liu, H Fang, W Tong. FDA-Approved Drug Labeling for the Study of Drug-Induced Liver Injury, Drug Discovery Today, 16(15-16):697-703, 2011. PMID:21624500 DOI:10.1016/j.drudis.2011.05.007 M Chen, A Suzuki, S Thakkar, K Yu, C Hu, W Tong. DILIRank: the largest reference drug list ranked by the risk for developing drug-induced liver injury in humans. Drug Discov Today 2016, 21(4): 648-653. PMID:26948801 DOI:10.1016/j.drudis.2016.02.015

▶ Drug Induced Liver Injury Rank (DILIRank) Dataset

13.1.3 Adverse Effects

?

Asthma - Reversible bronchoconstriction (narrowing of bronchioles) initiated by the inhalation of irritating or allergenic agents.

▶ Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

13.1.4 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 \(HSDB\)](#)

13.1.5 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 \(HSDB\)](#)

13.1.6 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 \(HSDB\)](#)

13.1.7 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:747722](#)

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](#) balance. /[Thiamine 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.

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

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

13.1.8 Non-Human Toxicity Values



LD50 Rat sc 560 mg/kg

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 \(HSDB\)](#)

LD50 Rat iv 188 mg/kg

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 \(HSDB\)](#)

LD50 Mouse sc 301 mg/kg

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 \(HSDB\)](#)

LD50 Mouse iv 83 mg/kg

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 \(HSDB\)](#)

13.1.9 Protein Binding

90-94%

▶ [DrugBank](#)

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; Thaimine (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

Food	Thiamine Content, ug/100g
Pork	600-950
Dried beans and whey	500
Nuts	300-560
Brown rice	300
Beef liver	300
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; Thiamine (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

Food	Serving	Vitamin B1 (mg)
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/infocenter/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 Sci. 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/infocenter/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/infocenter/vitamins/thiamin/index.html>

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

14 Associated Disorders and Diseases

► [Comparative Toxicogenomics Database \(CTD\)](#)

Associated Occupational Diseases with Exposure to the Compound

[Asthma, occupational](#) [Category: Airway Disease]

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

Disease	References
Hemodialysis	PubMed: 11684545 , 2013627 , 12092667 , 15353324 , 10838467 , 16221095 , 18085392 , 4002227 , 11325895 , 12738682 , 18045861 , 11380830
Friedreich's ataxia	PubMed: 1538220 , 11383938
Olivopontocerebral atrophy	PubMed: 1538220 , 11383938
Alcoholism	PubMed: 182198 , 15340856 , 11958947 , 16959481 , 2779169 , 9717263 , 3410397 , 8723414
Hereditary spastic paraplegia	PubMed: 11383938

Disease	References
Colorectal cancer	PubMed: 7482520 , 19006102 , 23940645 , 24424155 , 20156336 , 19678709 , 22148915 , 25105552 , 21773981 , 25037050 , 27015276 , 27107423 , 27275383 , 28587349 Silke Matysik, Caroline Ivanne Le Roy, Gerhard Liebisch, Sandrine Paule Claus. Metabolomics of fecal samples: A practical consideration. Trends in Food Science & Technology. Vol. 57, Part B, Nov. 2016, p.244-255: http://www.sciencedirect.com/science/article/pii/S0924224416301984

► [Human Metabolome Database \(HMDB\)](#)

15 Literature



15.1 Coronavirus Studies



► PubChem

15.2 NLM Curated PubMed Citations



► PubChem

15.3 Springer Nature References



► Springer Nature

15.4 Thieme References



► Thieme Chemistry

15.5 Wiley References



► Wiley

15.6 Depositor Provided PubMed Citations



► [PubChem](#)

15.7 Synthesis References



Nobuyuki Kitamori, Masaya Maeno, Seiji Izuhara, "Granules of thiamine salt and the production thereof." U.S. Patent US4702919, issued July, 1974.

► [DrugBank](#)

Sugimoto, Hirohiko; Ishiba, Teruyuki; Sato, Tomohiro; Nakai, Hiroshi; Hirai, Kentaro. Novel S-alkylation products from "isolated thiamin ylide" via thiaminium neothiaminethiolate ion pair. Journal of Organic Chemistry (1990), 55(2), 467-70.

► [Human Metabolome Database \(HMDB\)](#)

15.8 Metabolite References



► [Human Metabolome Database \(HMDB\)](#)

15.9 General References



1. Slater PV: Multi-level preparation for nursing impact on nursing practice. Aust Nurses J. 1978 Jun;7(11):40-3. [PMID:249270]
2. Kopriva V, Bilkovic R, Licko T: [Tumours of the small intestine (author's transl)]. Cesk Gastroenterol Vyz. 1977 Dec;31(8):549-53. [PMID:603941]
3. Beissel J: [The role of right catheterization in valvular prosthesis surveillance (author's transl)]. Ann **Cardiol** Angeiol (Paris). 1977 Dec;26(6):587-9. [PMID:606152]
4. Lonsdale D, Shamberger RJ, Audhya T: Treatment of autism spectrum children with **thiamine tetrahydrofurfuryl disulfide**: a pilot study. Neuro Endocrinol Lett. 2002 Aug;23(4):303-8. [PMID:12195231]
5. Lonsdale D: A review of the biochemistry, metabolism and clinical benefits of thiamin(e) and its derivatives. Evid Based Complement Alternat Med. 2006 Mar;3(1):49-59. [PMID:16550223]

► [DrugBank](#)

Jenkins et al. A New Thiamin Salvage Pathway. Nature Chemical Biology, doi: 10.1038/NChemBio.2007.13, published online 8 July 2007.
<http://www.nature.com/naturechemicalbiology>

► [Nature Chemical Biology](#)

Chatterjee et al. Reconstitution of ThiC in thiamine pyrimidine biosynthesis expands the radical SAM superfamily Nature Chemical Biology, doi: 10.1038/nchembio.121, published online 26 October 2008 <http://www.nature.com/naturechemicalbiology>

► [Nature Chemical Biology](#)

15.10 Chemical Co-Occurrences in Literature



► PubChem

15.11 Chemical-Gene Co-Occurrences in Literature



► PubChem

15.12 Chemical-Disease Co-Occurrences in Literature



► PubChem

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=NRFUQFSJQZTSJH-UHFFFAOYSA-N>

► PATENTSCOPE (WIPO)

Patents are available for this chemical structure:

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

► PATENTSCOPE (WIPO)

17 Interactions and Pathways



17.1 Protein Bound 3D Structures



► [RCSB Protein Data Bank \(RCSB PDB\)](#)

[View 12 proteins in NCBI Structure](#)

► [PubChem](#)

17.1.1 Ligands from Protein Bound 3D Structures



PDBe Ligand Code	VIB
PDBe Structure Code	1IG3
PDBe Conformer	

► [Protein Data Bank in Europe \(PDBe\)](#)

17.2 Chemical-Target Interactions



► BindingDB

► Comparative Toxicogenomics Database (CTD)

► [DrugBank](#)

► [IUPHAR/BPS Guide to PHARMACOLOGY](#)

► Therapeutic Target Database (TTD)

17.3 Drug-Drug Interactions



► DrugBank

17.4 Pathways



► PubChem

18 Biological Test Results



18.1 BioAssay Results



► PubChem

19 Taxonomy



Thiamine is a metabolite found in or produced by [Escherichia coli \(strain K12, MG1655\)](#).

► [E. coli Metabolome Database \(ECMDB\)](#)

WormJam Metabolites Local CSV for MetFrag | [DOI:10.5281/zenodo.3403364](#)

WormJam: A consensus C. elegans Metabolic Reconstruction and Metabolomics Community and Workshop Series, Worm, 6:2, e1373939, DOI:10.1080/21624054.2017.1373939

► [ECI Group, LCSB, University of Luxembourg](#)

The LOTUS Initiative for Open Natural Products Research: frozen dataset union wikidata (with metadata) | [DOI:10.5281/zenodo.5794106](https://doi.org/10.5281/zenodo.5794106)

► [LOTUS - the natural products occurrence database](#)

Thiamine is a metabolite found in or produced by [Saccharomyces cerevisiae](#).

► [Yeast Metabolome Database \(YMDB\)](#)

20 Classification



20.1 MeSH Tree



► Medical Subject Headings (MeSH)

20.2 ChEBI Ontology



[▶ ChEBI](#)

20.3 KEGG: Metabolite

[▶ KEGG](#)

20.4 WHO ATC Classification System



► WHO Anatomical Therapeutic Chemical (ATC) Classification

20.5 ChemIDplus



► ChemIDplus

20.6 IUPHAR/BPS Guide to PHARMACOLOGY Target Classification



► IUPHAR/BPS Guide to PHARMACOLOGY

20.7 ChEMBL Target Tree



► ChEMBL

20.8 NORMAN Suspect List Exchange Classification



► NORMAN Suspect List Exchange

20.9 CCSBase Classification



► CCSbase

20.10 EPA DSSTox Classification



▶ EPA DSSTox

20.11 LOTUS Tree



▶ LOTUS - the natural products occurrence database

20.12 FDA Drug Type and Pharmacologic Classification



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

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Thiamine

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<https://www.guidetopharmacology.org/GRAC/LigandDisplayForward?ligandId=4628>

Guide to Pharmacology Target Classification

<https://www.guidetopharmacology.org/targets.jsp>

5. Therapeutic Target Database (TTD)

[3H]thiamine

<http://idrblab.net/ttd/data/drug/details/D07TYL>

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3-[(4-Amino-2-methyl-5-pyrimidinyl)methyl]-5-(2-hydroxyethyl)-4-methylthiazolium
https://commonchemistry.cas.org/detail?cas_rn=70-16-6

7. ChemIDplus

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<https://chem.nlm.nih.gov/chemidplus/sid/0000070166>

ChemIDplus Chemical Information Classification

<https://chem.nlm.nih.gov/chemidplus/>

8. EPA DSSTox

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

Thiamine ion

<https://comptox.epa.gov/dashboard/DTXSID50220251>

CompTox Chemicals Dashboard Chemical Lists

<https://comptox.epa.gov/dashboard/chemical-lists/>

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Thiamine

<https://echa.europa.eu/substance-information/-/substanceinfo/100.000.387>

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THIAMINE ION

<https://gsrs.ncats.nih.gov/ginas/app/beta/substances/4ABT0J945J>

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

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<http://www.hmdb.ca/metabolites/HMDB0000235>

HMDB0000235_nmr_one_1211

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Thiamine

CCSbase Classification

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NORMAN Suspect List Exchange Classification

<https://www.norman-network.com/nds/SLE/>

15. ChEBI

Thiamine(1+)

<http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:18385>

ChEBI Ontology

<http://www.ebi.ac.uk/chebi/userManualForward.do#ChEBI%20Ontology>

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LOTUS Tree

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Thiamine

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thiamine

<https://www.fda.gov/science-research/liver-toxicity-knowledge-base-ltkb/drug-induced-liver-injury-rank-dilirank-dataset>

24. Nature Chemical Biology

<https://pubchem.ncbi.nlm.nih.gov/substance/24775656>

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

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<https://www.fda.gov/drugs/drug-approvals-and-databases/approved-drug-products-therapeutic-equivalence-evaluations-orange-book>

29. **SpectraBase**

Thiamin

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

Thiamine cation

<https://spectrabase.com/spectrum/H9C3wvYRtfc>

Thiamin

<https://spectrabase.com/spectrum/8HRQmkYquS5>

Thiamine ,salt; Thiamine cation

<https://spectrabase.com/spectrum/87zLfvGODqw>

THIAMINE

<https://spectrabase.com/spectrum/9PeLksARlfB>

2-[3-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-4-methyl-5-thiazol-3-iumyl]ethanol

<https://spectrabase.com/spectrum/9qyugfp2B6>

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<https://markerdb.ca/>

Thiamine

<https://markerdb.ca/chemicals/151>

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JZRWCGZRTZMZEH-UHFFFAOYSA-N

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thiamine ion

<https://rxnav.nlm.nih.gov/id/rxnorm/1546268>

35. Protein Data Bank in Europe (PDBe)

<http://www.ebi.ac.uk/pdbe-srv/pdbechem/chemicalCompound/show/VIB>

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MeSH Tree

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Vitamin B Complex

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