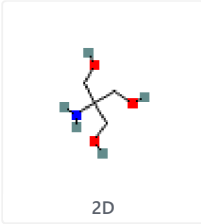
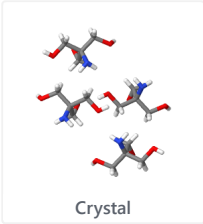
PubChem

COMPOUND SUMMARY

Tromethamine

PubChem CID:	6503
Structure:	 2D  3D  Crystal Find Similar Structures
Chemical Safety:	 Irritant Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula:	$C_4H_{11}NO_3$
Chemical Names:	Trometamol 77-86-1 TROMETHAMINE Tris Tris(Hydroxymethyl)aminomethane More...
Molecular Weight:	121.14 g/mol
Dates:	Modify: 2019-08-10 Create: 2005-03-26

Tris is a primary amino compound that is tert-butylamine in which one hydrogen attached to each

Cite Download

CONTENTS

methyl group is replaced by a hydroxy group. A compound widely used as a biological buffer substance in the pH range 7--9; pKa = 8.3 at 20 degreeC; pKa = 7.82 at 37 degreeC. It has a role as a buffer. It is a triol and a primary amino compound. It is a conjugate base of a member of Htris.

▶ from ChEBI

An organic amine proton acceptor. It is used in the synthesis of surface-active agents and pharmaceuticals; as an emulsifying agent for cosmetic creams and lotions, mineral oil and paraffin wax emulsions, as a biological buffer, and used as an alkalizer. (From Merck, 11th ed; Martindale, The Extra Pharmacopoeia, 30th ed, p1424)

▶ from DrugBank

Tromethamine, also known as trometamol or tham, belongs to the class of organic compounds known as 1, 2-aminoalcohols. These are organic compounds containing an alkyl chain with an amine group bound to the C1 atom and an alcohol group bound to the C2 atom. Tromethamine is a drug which is used for the prevention and correction of metabolic acidosis. Tromethamine exists as a solid, soluble (in water), and a very weakly acidic compound (based on its pKa). Tromethamine is also a parent compound for other transformation products, including but not limited to, bis-tris, bis-tris propane, and N-tris(hydroxymethyl)methylglycine.

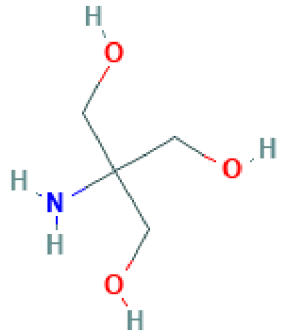
▶ from Human Metabolome Database (HMDB)

1 Structures

1.1 2D Structure

Find Similar Structures | Get Image | Download

Chemical Structure Depiction



from PubChem

1.2 3D Conformer

from PubChem

1.3 Crystal Structures

Showing 1 of 6 View More

CCDC Number	128604
Crystal Structure Data	DOI:10.5517/cc49tjr
Crystal Structure Depiction	
Associated Article	DOI:10.1107/S0108270196013649

from The Cambridge Structural Database

2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

2-amino-2-(hydroxymethyl)propane-1,3-diol

from PubChem

2.1.2 InChI

InChI=1S/C4H11NO3/c5-4(1-6,2-7)3-8/h6-8H,1-3,5H2

from PubChem

2.1.3 InChI Key

LENZDBCJOHFCAS-UHFFFAOYSA-N

from PubChem

2.1.4 Canonical SMILES

C(C(CO)(CO)N)O

from PubChem

2.2 Molecular Formula

$C_4H_{11}NO_3$

from PubChem

2.3 Other Identifiers

2.3.1 CAS

77-86-1

from ChemIDplus; DrugBank; DTP/NCI; EPA Chemicals under the TSCA; EPA DSSTox; European Chemicals Agency (ECHA)

Other CAS

108195-86-4

25149-07-9

68755-45-3

83147-39-1

119320-15-9

857365-23-2

1158650-64-6

- from ChemIDplus

2.3.2 European Community (EC) Number

201-064-4

- from European Chemicals Agency (ECHA)

2.3.3 NSC Number

65434

- from DTP/NCI

6365

- from DTP/NCI

2.3.4 UNII

023C2WHX2V

- from FDA/SPL Indexing Data

2.3.5 Wikipedia

Tromethamine

- from Wikipedia

2.4 Synonyms

2.4.1 MeSH Entry Terms

Tri(hydroxymethyl)aminomethane

Tris Buffer

Tris(hydroxymethyl)aminomethane

Tris-Magnesium(II)-Potassium Chloride Buffer

Tris-Mg(II)-KCl Buffer

Trisamine

Trizma

Trometamol

Tromethamine

▸ from MeSH

2.4.2 Depositor-Supplied Synonyms

Trometamol

77-86-1

TROMETHAMINE

Tris

Tris(Hydroxymethyl)aminomethane

Tham

Trisamine

2-Amino-2-(hydroxymethyl)-1,3-propanediol

2-Amino-2-(hydroxymethyl)propane-1,3-diol

Trizma

Tris buffer

Tris base

Trisaminol

Tromethane

Pehanorm

Talatrol

Trisamin

- Trispuffer
- Tutofusin tris
- Apiroserum Tham
- Tris-steril
- Addex-tham
- Tris-base
- Tris, free base
- Trimethylolaminomethane
- 1,3-Propanediol, 2-amino-2-(hydroxymethyl)-
- Tris Amino
- Aminotrimethylolmethane
- Aminotris(hydroxymethyl)methane
- THAM-E
- Tris (buffering agent)
- Tromethanmin
- Tris(hydroxymethyl)methylamine
- Tris(hydroxymethyl)methanamine
- Trometamole
- Tromethamolum
- Trizma base
- Tri(hydroxymethyl)aminomethane
- 2-Amino-2-methylol-1,3-propanediol
- Tris-hydroxymethylaminomethane
- Caswell No. 036
- 2-Amino-2-hydroxymethyl-1,3-propanediol
- Tris-Amino
- Methylamine, 1,1,1-tris(hydroxymethyl)-
- Trometamolum [INN-Latin]
- NSC 6365
- 2-(Hydroxymethyl)-2-amino-1,3-propanediol

UNII-023C2WHX2V

Tris-hydroxymethyl-aminomethan

Methanamine, 1,1,1-tris(hydroxymethyl)-

HSDB 3408

EINECS 201-064-4

MFCD00004679

EPA Pesticide Chemical Code 083901

Tris-hydroxymethyl-aminomethan [German]

AI3-03948

023C2WHX2V

CHEBI:9754

Tris(Hydroxymethyl)-Aminomethane

Tris(hydroxymethyly)amino methane

Tris-(hydroxymethyl)-aminomethane

NSC6365

LENZDBCJOHFCAS-UHFFFAOYSA-N

1,1,1-tris(hydroxymethyl)methanamine

TRIS (tromethamine)

NCGC00159412-02

NCGC00159412-04

Tris buffertris-hydroxymethyl-aminomethan

TRIS, ULTRA PURE

DSSTox_CID_3723

trishydroxymethylaminomethane

WLN: Q1XZ1Q1Q

DSSTox_RID_77165

2-Amino-2-hydroxymethyl-1,3-propanediol solution

DSSTox_GSID_23723

Trometamolum

1, 2-amino-2-(hydroxymethyl)-

Triladyl

Trigmo base

MFCD00132476

Methanamine,1,1-tris(hydroxymethyl)-

Methylamine,1,1-tris(hydroxymethyl)-

tris(hydroxymethyl)amino methane

CAS-77-86-1

Tris(hydroxymethyl)aminomethane, >=99.8%

Tromethamine [USAN]

2-amino-2-(hydroxymethyl)-1, 3-propanediol

Tris(hydroxymethyl)aminomethane, Electrophoresis Grade

Tris-Mg(II)-KCl Buffer

Tromethamine [USAN:USP]

Tris(hydroxymethyl)aminomethane, 99+%, for biochemistry

Trometamina

Tromethamin

Aminotri(hydroxymethyl)methane

Tribase

Trometamol, Tromethamine, Tris-[hydroxymethyl]amino- methane

tris-amine

TrizmaTM

Tro.meta.mole

Tris(hydroxymethyl)aminomethane, 99.8%, for analysis, biochemical grade

Tro.meta.mol

1gng

83147-39-1

Tris(hydroxymethyl)aminomethane, 99.85%, for molecular biology, DNAse, RNAse and Protease free

Trometamol [INN]

Tromethamine (USP)

TRIS Ultrapure, EP

- 1h4n
- Trometamol (JAN/INN)
- AC1L1MOA
- TRS
- Tris-Magnesium(II)-Potassium Chloride Buffer
- SCHEMBL975
- trishydroxymethylmethylamine
- THAM (TN)
- Buffer Salt, pH 10.5
- EC 201-064-4
- Tri(hydroxymethyl)methylamin
- NCIOpen2_000263
- NCIOpen2_001720
- Oprea1_677781
- TRIS, U.S.P.
- trishydroxymethyl aminomethane
- tris-hydroxymethyl-methylamine
- B-TRIS500
- MLS000028643
- ARONIS23912
- tris hydroxymethyl aminomethane
- Tris (hydroxymethyl)aminoethane
- AC1Q50D3
- AC1Q50D4
- GTPL7328
- tris (hydroxymethyl)aminomethane
- tris(hydroxymethyl) aminomethane
- CHEMBL1200391
- DTXSID2023723
- tris (hydroxymethyl) methylamine

Tris-[hydroxymethyl]amino-methane

2-Amino-2-hydroxymethylpropanediol

HMS3652L05

tris-(hydroxymethyl)-amino-methane

ZINC896695

BCP05578

KS-000002LE

NSC-6365

NSC65434

Tox21_111645

Tox21_201646

Tox21_303167

BBL000011

NSC-65434

s4176

SBB006714

STK379529

2-amino-2-methylol-propane-1,3-diol

AKOS000121321

Tox21_111645_1

AM90366

CCG-214012

CS-W018524

DB03754

MCULE-7300085951

NE10342

RP19408

Trizma(R) base, >=99.0% (T)

ATX Tris buffer, ready-to-use solution

Tris(hydroxymethyl)aminomethane, >=99%

NCGC00159412-03

NCGC00159412-05

NCGC00257164-01

NCGC00259195-01

TRIS, 0.5M buffer solution, pH 6.8

TRIS, 0.5M buffer solution, pH 7.2

TRIS, 0.5M buffer solution, pH 7.4

TRIS, 0.5M buffer solution, pH 7.5

TRIS, 0.5M buffer solution, pH 8.0

TRIS, 0.5M buffer solution, pH 8.5

TRIS, 0.5M buffer solution, pH 8.6

TRIS, 0.5M buffer solution, pH 8.8

TRIS, 0.5M buffer solution, pH 9.0

TRIS, 0.5M buffer solution, pH 9.5

TRIS, 1.0M buffer solution, pH 6.5

TRIS, 1.0M buffer solution, pH 7.4

TRIS, 1.0M buffer solution, pH 7.6

TRIS, 1.0M buffer solution, pH 7.8

TRIS, 1.0M buffer solution, pH 8.2

TRIS, 1.0M buffer solution, pH 8.4

TRIS, 1.0M buffer solution, pH 8.6

TRIS, 1.0M buffer solution, pH 8.8

TRIS, 1.0M buffer solution, pH 9.0

AJ-24245

AK-41163

AN-23925

BP-13394

SC-44694

SMR000059179

Tris(hydroxymethyl)aminomethane ACS grade

Tris(hydroxymethyl)aminomethane, ultrapure

2-amino-2-[hydroxymethyl]-1,3-propandiol

AB1002112

LS-120135

Methanamine, 1, 1,1-tris(hydroxymethyl)-

TL8005336

Tris acidimetric, NIST(R) SRM(R) 723e

A0321

FT-0611014

ST24027700

ST51037436

SW219208-1

T6977

TRIS-buffered saline (TBS, 10X) pH 7.4

TRIS-buffered saline (TBS, 10X) pH 7.6

TRIS-buffered saline (TBS, 10X) pH 8.0

TRIS-buffered saline (TBS, 20X) pH 7.4

2-(Hydroxymethyl)-2-amino-1, 3-propanediol

2-amino-2-(hydroxyl-methyl)propane-1,3-diol

2-amino-2-(hydroxymethyl) propane-1,3-diol

Tris-amino, Tromethane, Trometamol, Trisamine

Trizma(R) base, BioUltra, >=99.8% (T)

Trizma(R) base, tested according to Ph.Eur.

Tromethamine, meets USP testing specifications

1606-EP1441224A2

1606-EP2269977A2

1606-EP2269992A1

1606-EP2270000A1

1606-EP2270001A1

1606-EP2270004A1

1606-EP2270014A1

1606-EP2270101A1

1606-EP2270895A2

1606-EP2272516A2

1606-EP2272817A1

1606-EP2272825A2

1606-EP2272827A1

1606-EP2272835A1

1606-EP2272844A1

1606-EP2272972A1

1606-EP2272973A1

1606-EP2275105A1

1606-EP2275413A1

1606-EP2275420A1

1606-EP2275469A1

1606-EP2277507A1

1606-EP2277872A1

1606-EP2277877A1

1606-EP2277881A1

1606-EP2277882A1

1606-EP2278637A1

1606-EP2280004A1

1606-EP2280005A1

1606-EP2280006A1

1606-EP2280011A1

1606-EP2280012A2

1606-EP2280020A1

1606-EP2280021A1

1606-EP2281813A1

1606-EP2281818A1

1606-EP2281899A2

1606-EP2284157A1

1606-EP2284169A1

1606-EP2286795A1

1606-EP2287156A1

1606-EP2287161A1

1606-EP2287162A1

1606-EP2287165A2

1606-EP2287166A2

1606-EP2289868A1

1606-EP2289883A1

1606-EP2289884A1

1606-EP2289886A1

1606-EP2289890A1

1606-EP2289891A2

1606-EP2289894A2

1606-EP2292589A1

1606-EP2292593A2

1606-EP2292596A2

1606-EP2292607A2

1606-EP2292610A1

1606-EP2292620A2

1606-EP2295055A2

1606-EP2295406A1

1606-EP2295410A1

1606-EP2295417A1

1606-EP2295421A1

1606-EP2295423A1

1606-EP2295424A1

1606-EP2295429A1

1606-EP2295434A2

1606-EP2295436A1

1606-EP2295439A1

1606-EP2295550A2

1606-EP2298305A1

1606-EP2298312A1

1606-EP2298728A1

1606-EP2298744A2

1606-EP2298769A1

1606-EP2298773A1

1606-EP2298774A1

1606-EP2298783A1

1606-EP2299785A1

1606-EP2301921A1

1606-EP2301926A1

1606-EP2301928A1

1606-EP2301930A1

1606-EP2301932A1

1606-EP2301934A1

1606-EP2301937A1

1606-EP2301939A1

1606-EP2302382A2

1606-EP2302383A2

1606-EP2305250A1

1606-EP2305641A1

1606-EP2305672A1

1606-EP2305677A1

1606-EP2305687A1

1606-EP2305825A1

1606-EP2306788A1

1606-EP2306789A1

1606-EP2308841A2

1606-EP2308851A1

1606-EP2308855A1

1606-EP2308866A1

1606-EP2308873A1

1606-EP2308874A1

1606-EP2308878A2

1606-EP2311453A1

1606-EP2311801A1

1606-EP2311802A1

1606-EP2311803A1

1606-EP2311807A1

1606-EP2311814A1

1606-EP2311818A1

1606-EP2314571A2

1606-EP2314584A1

1606-EP2314585A1

1606-EP2316824A1

1606-EP2316830A2

1606-EP2316832A1

1606-EP2316833A1

1606-EP2371811A2

1606-EP2371814A1

1606-EP2374784A1

1606-EP2374785A1

3368-EP2269610A2

3368-EP2270002A1

3368-EP2270010A1

3368-EP2272517A1

3368-EP2272822A1

3368-EP2277848A1

3368-EP2281815A1

3368-EP2284160A1

3368-EP2284172A1

3368-EP2289510A1

3368-EP2289890A1

3368-EP2295406A1

3368-EP2295409A1

3368-EP2301933A1

3368-EP2301937A1

3368-EP2305250A1

3368-EP2305640A2

3368-EP2305646A1

3368-EP2305677A1

3368-EP2305679A1

3368-EP2305682A1

3368-EP2308840A1

3368-EP2308879A1

3368-EP2311827A1

3368-EP2311842A2

3368-EP2314295A1

3368-EP2314574A1

3368-EP2314588A1

3368-EP2314590A1

3368-EP2316457A1

3368-EP2316458A1

3368-EP2316825A1

3368-EP2316826A1

3368-EP2316827A1

3368-EP2316828A1

C07182

D00396

M02623

23153-EP2270505A1

23153-EP2272832A1

23153-EP2281899A2

23153-EP2284159A1

23153-EP2287163A1

23153-EP2289883A1

23153-EP2292592A1

23153-EP2295407A1

23153-EP2298736A1

23153-EP2298743A1

23153-EP2298767A1

23153-EP2298778A1

23153-EP2305641A1

23153-EP2305651A1

23153-EP2305678A1

23153-EP2305684A1

23153-EP2308510A1

23153-EP2308854A1

23153-EP2314584A1

23153-EP2314587A1

27256-EP2272822A1

27256-EP2314575A1

42340-EP2305808A1

42340-EP2308479A2

42340-EP2311808A1

42340-EP2311829A1

AB00443859_03

AB00443859_04

111860-EP2292611A1

111860-EP2298761A1

116174-EP2289891A2

116174-EP2298770A1

Sigma 7-9(R), >=99% (titration), crystalline

SR-01000944234

Trizma(R) base, puriss. p.a., >=99.7% (T)

I14-0997

J-610076

SR-01000944234-1

Trizma(R) base, >=99.9% (titration), crystalline

Trizma(R) base, Vetec(TM) reagent grade, >=99%

W-104296

Tris(hydroxymethyl)aminomethane, 99.8%, ACS reagent

Tris(hydroxymethyl)aminomethane, ACS reagent, 99.9%

TRIS-buffered saline (TBS, 10X, low salt) pH 8.0

F0001-1979

Tris(hydroxymethyl)aminomethane, ACS reagent, >=99.8%

Tris(hydroxymethyl)aminomethane, Molecular Biology Grade

TRIS-buffered saline (TBS, 10X, high salt) pH 7.4

Z1317839150

Tris(hydroxymethyl)aminomethane, p.a., ACS reagent, 99.8%

Tris(hydroxymethyl)aminomethane, ultrapure grade, >=99.9%

TRIS-buffered saline (TBS, 10X), with 1% Triton X-100

Trizma(R) base, puriss. p.a., buffer substance, >=99.5%

Trometamol, European Pharmacopoeia (EP) Reference Standard

Trometamol, Tromethamine, Tris-[hydroxymethyl]amino-methane

Tris(hydroxymethyl)aminomethane, JIS special grade, >=99.0%

Tris(hydroxymethyl)aminomethane; THAM; Tris base; Trometamol

TRIS, 1.0M buffer solution, pH 7.0, 0.2 micron filtered

TRIS, 1.0M buffer solution, pH 8.5, 0.2 micron filtered

TRIS, 1.0M buffer solution, pH 9.0, 0.2 micron filtered

TRIS-buffered saline (TBS, 10X) pH 7.4, for Western blot

InChI=1/C4H11NO3/c5-4(1-6,2-7)3-8/h6-8H,1-3,5H

Trizma(R) base, anhydrous, free-flowing, Redi-Dri(TM), >=99.9%

Trizma(R) base, BioUltra, for molecular biology, >=99.8% (T)

Tromethamine, United States Pharmacopeia (USP) Reference Standard

Trizma(R) base, cell culture tested, >=99.9% (titration), crystalline

Trizma(R) base, BioXtra, pH 10.5-12.0 (1 M in H2O), >=99.9% (titration)

Trizma(R) base, Primary Standard and Buffer, >=99.9% (titration), crystalline

Tromethamine, Pharmaceutical Secondary Standard; Certified Reference Material

Trizma(R) base, BioPerformance Certified, meets EP, USP testing specifications, cell culture tested, >=99.9% (titration)

Trizma(R) base, certified reference material for titrimetry, certified by BAM, according to ISO 17025, >=99.5%

Tromethamine, PharmaGrade, Manufactured under appropriate controls for use as a raw material in pharma or biopharmaceutical production, suitable for cell culture, Meets USP, EP, JPC, BP testing specifications.

Tromethamine, PharmaGrade, Manufactured under appropriate controls for use as a raw material in pharma or biopharmaceutical production., suitable for cell culture, meets USP testing specifications

▶ from PubChem

3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value
Molecular Weight	121.14 g/mol
XLogP3-AA	-2.9

Property Name	Property Value
Hydrogen Bond Donor Count	4
Hydrogen Bond Acceptor Count	4
Rotatable Bond Count	3
Exact Mass	121.073893 g/mol
Monoisotopic Mass	121.073893 g/mol
Topological Polar Surface Area	86.7 A^2
Heavy Atom Count	8
Formal Charge	0
Complexity	54
Isotope Atom Count	0
Defined Atom Stereocenter Count	0
Undefined Atom Stereocenter Count	0
Defined Bond Stereocenter Count	0
Undefined Bond Stereocenter Count	0
Covalently-Bonded Unit Count	1
Compound Is Canonicalized	Yes

from PubChem

3.2 Experimental Properties

3.2.1 Physical Description

Liquid

from EPA Chemicals under the TSCA

3.2.2 Color/Form

Crystalline mass

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 1677

from HSDB

WHITE, CRYSTALLINE POWDER

Osol, A. and J.E. Hoover, et al. (eds.). Remington's Pharmaceutical Sciences. 15th ed. Easton, Pennsylvania: Mack Publishing Co., 1975., p. 773

from HSDB

3.2.3 Odor

SLIGHT, CHARACTERISTIC ODOR

Osol, A. and J.E. Hoover, et al. (eds.). Remington's Pharmaceutical Sciences. 15th ed. Easton, Pennsylvania: Mack Publishing Co., 1975., p. 773

from HSDB

3.2.4 Taste

FAINT, SWEET, SOAPY TASTE

Osol, A. and J.E. Hoover, et al. (eds.). Remington's Pharmaceutical Sciences. 15th ed. Easton, Pennsylvania: Mack Publishing Co., 1975., p. 773

from HSDB

3.2.5 Boiling Point

219-220 deg C at 10 mm Hg

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 1677

from HSDB

3.2.6 Melting Point

171-172 deg C

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 1677

from HSDB

3.2.7 Solubility

79.1 mg/mL in ethylene glycol; 26 mg/mL in methanol; 14.6 mg/mL in anhyd ethanol; 22 mg/mL in 95% ethanol; 14 mg/mL in dimethyl formamide; 20 mg/mL in acetone; 0.5 mg/mL in ethyl acetate; 0.4 mg/mL in olive oil; 0.1 mg/mL in cyclohexane; 0.05 mg/mL in chloroform; less than 0.05 mg/mL in carbon tetrachloride

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 1677

from HSDB

In water, 5.50X10+5 mg/L at 25 deg C

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 1677

from HSDB

3.2.8 Vapor Pressure

2.2X10-5 mm Hg at 25 deg C (est)

US EPA; Estimation Program Interface (EPI) Suite. Ver.3.20. February, 2007. Available from, as of Dec 7, 2007: ***http://www.epa.gov/oppt/exposure/pubs/episuitedl.htm***

from HSDB

3.2.9 Octanol/Water Partition Coefficient

log Kow = -1.56 (est)

US EPA; Estimation Program Interface (EPI) Suite. Ver.3.20. February, 2007. Available from, as of Dec 7, 2007: ***http://www.epa.gov/oppt/exposure/pubs/episuitedl.htm***

from HSDB

3.2.10 Stability/Shelf Life

Stable in light and air

Osol, A. and J.E. Hoover, et al. (eds.). Remington's Pharmaceutical Sciences. 15th ed. Easton, Pennsylvania: Mack Publishing Co., 1975., p. 773

from HSDB

3.2.11 Decomposition

When heated to decomposition it emits toxic fumes of /nitrogen oxide/.

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 3436

from HSDB

3.2.12 pH

pH of 0.1 molar aq soln = 10.4

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 1677

from HSDB

3.2.13 Dissociation Constants

pKa = 8.07

Perinn DD; Dissociation Constants of Organic Bases in Aqueous Solution. IUPAC Chem Data Ser: Suppl 1972. London, England: Buttersworth (1972)

from HSDB

3.2.14 Kovats Retention Index

Standard non-polar	1645

from NIST

3.2.15 Other Experimental Properties

Weak, monoacidic base; aq soln do not absorb CO2 from air

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 1677

from HSDB

REACTS WITH PROTON DONORS

Osol, A. and J.E. Hoover, et al. (eds.). Remington's Pharmaceutical Sciences. 15th ed. Easton, Pennsylvania: Mack Publishing Co., 1975., p. 773

from HSDB

Henry's Law constant = 8.7X10-13 atm-cu m/mol at 25 deg C (est)

US EPA; Estimation Program Interface (EPI) Suite. Ver.3.20. February, 2007. Available from, as of Dec 7, 2007: ***http://www.epa.gov/oppt/exposure/pubs/episuitedl.htm***

from HSDB

Hydroxyl radical reaction rate constant = 3.4X10-11 cu cm/molecule-sec at 25 deg C (est)

US EPA; Estimation Program Interface (EPI) Suite. Ver.3.20. February, 2007. Available from, as of Dec 7, 2007: ***http://www.epa.gov/oppt/exposure/pubs/episuitedl.htm***

from HSDB

4 Spectral Information

4.1 1D NMR Spectra

1D NMR Spectra	NMR: 6342 (Sadtler Research Laboratories Spectral Collection)

from HSDB

1D NMR Spectra	NMRShiftDB Link

from NMRShiftDB

4.1.1 1H NMR Spectra

Instrument Name	BRUKER AC-300
Source of Sample	Tokyo Kasei Kogyo Company, Ltd., Tokyo, Japan

Copyright	Copyright © 1991-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

from SpectraBase

Instrument Name	Varian A-60
Source of Sample	Aldrich Chemical Company, Inc., Milwaukee, Wisconsin
Copyright	Copyright © 2009-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

▶ from SpectraBase

4.1.2 13C NMR Spectra

Source of Sample	Chem Service, Inc., West Chester, Pennsylvania
Copyright	Copyright © 1980, 1981-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

▶ from SpectraBase

Copyright	Copyright © 2016 W. Robien, Inst. of Org. Chem., Univ. of Vienna. All Rights Reserved.
Thumbnail	

from SpectraBase

4.2 Mass Spectrometry

Showing 2 of 6 View More

Mass Spectrometry	MASS: 69526 (NIST/EPA/MSDC Mass SPectral database, 1990 version)

from HSDB

MoNA ID	KO002368
MS Category	Experimental
MS Type	Chromatography identified as LC-MS
MS Level	MS2
Precursor Type	[M+H]+
precursor m/z	122
Instrument	API3000, Applied Biosystems
Instrument Type	LC-ESI-QQ
Ionization Mode	positive
Collision Energy	10 V
Splash	splash10-00di-0900000000-53da6b0f35ab1e8e8a57
Thumbnail	

Submitter	Yuji Kakazu, Institute for Advanced Biosciences, Keio University

from MassBank of North America (MoNA)

4.2.1 GC-MS

Showing 2 of 3 View More

NIST Number	229605
Library	Main library
Total Peaks	50
m/z Top Peak	90
m/z 2nd Highest	60
m/z 3rd Highest	42
Thumbnail	

from NIST

NIST Number	221178
Library	Replicate library
Total Peaks	36
m/z Top Peak	90
m/z 2nd Highest	60
m/z 3rd Highest	30
Thumbnail	

from NIST

4.2.2 MS-MS

MS-MS	MS-MS Spectrum 59346 - HMDB HMDB0240288 MS-MS Spectrum 59347 - HMDB HMDB0240288 MS-MS Spectrum 59348 - HMDB HMDB0240288 MS-MS Spectrum 115464 - HMDB HMDB0240288 MS-MS Spectrum 115465 - HMDB HMDB0240288 MS-MS Spectrum 115466 - HMDB HMDB0240288 MS-MS Spectrum 445751 - HMDB HMDB0240288

	MS-MS Spectrum 445752 - HMDB HMDB0240288 MS-MS Spectrum 445753 - HMDB HMDB0240288 MS-MS Spectrum 445754 - HMDB HMDB0240288 MS-MS Spectrum 445755 - HMDB HMDB0240288

▸ from Human Metabolome Database (HMDB)

NIST Number	1118795
Instrument Type	IT/ion trap
Collision Energy	0
Spectrum Type	MS2
Precursor Type	[M+H]+
Precursor m/z	122.0812
Total Peaks	6
m/z Top Peak	104.2
m/z 2nd Highest	56.2
m/z 3rd Highest	122.2
Thumbnail	

▸ from NIST

4.3 IR Spectra

IR Spectra	IR: 5998 (Coblentz Society Spectral Collection)

▸ from HSDB

4.3.1 FTIR Spectra

Technique	KBr WAFER
Source of Sample	Polysciences, Inc., Warrington, Pennsylvania
Copyright	Copyright © 1980, 1981-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

▸ from SpectraBase

Technique	KBr WAFER
Source of Sample	Aldrich Chemical Company, Inc., Milwaukee, Wisconsin
Copyright	Copyright © 1980, 1981-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

from SpectraBase

4.3.2 ATR-IR Spectra

Instrument Name	Bruker Tensor 27 FT-IR
Technique	ATR-Neat (DuraSamplIR II)
Source of Spectrum	Bio-Rad Laboratories, Inc.
Source of Sample	Sigma-Aldrich Company Llc.
Catalog Number	T1503
Lot Number	SLBB6102V
Copyright	Copyright © 2014-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

from SpectraBase

4.4 Raman Spectra

Instrument Name	Bio-Rad FTS 175C with Raman accessory
Technique	FT-Raman
Source of Sample	Polysciences, Inc., Warrington, Pennsylvania
Copyright	Copyright © 1980, 1981-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

from SpectraBase

5 Related Records

5.1 Related Compounds with Annotation

from PubChem

5.2 Related Compounds

Same Connectivity	6 Records
Same Parent, Connectivity	98 Records
Same Parent, Exact	93 Records
Mixtures, Components, and Neutralized Forms	1,625 Records
Similar Compounds	43 Records
Similar Conformers	509 Records

from PubChem

5.3 Substances

5.3.1 Related Substances

All	5,236 Records
Same	1,639 Records
Mixture	3,597 Records

from PubChem

5.3.2 Substances by Category

from PubChem

5.4 Entrez Crosslinks

PubMed	14,286 Records
Protein Structures	1,160 Records
Taxonomy	1 Record
Gene	1 Record

from PubChem

5.5 NCBI LinkOut

from NCBI

6 Chemical Vendors

from PubChem

7 Drug and Medication Information

7.1 Drug Indication

For the prevention and correction of metabolic acidosis.

- from DrugBank

FDA Label

- from DrugBank

7.2 FDA Orange Book

- from FDA Orange Book

7.3 Drug Labels for Ingredients

Label Information	Total 151 labels
Drug Ingredient	TROMETHAMINE
NDC Code(s)	0009-0856-05, 0009-0856-08, 0023-2181-05, 0023-3507-05, 0023-3507-30, 0023-3507-31, 0023-9277-05, 0065-0345-10, 0093-0314-01, 0338-0069-10 ... total 362.
Packagers	A-S Medication Solutions; Aidarex Pharmaceuticals LLC; Akorn; Akorn Inc.; Alcon Laboratories, Inc.; Allergan, Inc.; Alvogen Inc.; American Regent, Inc.; Amphastar Pharmaceuticals, Inc.; Apotex Corp. ... total 75.

from DailyMed

7.4 Clinical Trials

7.4.1 ClinicalTrials.gov

from ClinicalTrials.gov

7.4.2 EU Clinical Trials Register

from EU Clinical Trials Register

7.4.3 NIPH Clinical Trials Search of Japan

from NIPH Clinical Trials Search of Japan

7.5 Therapeutic Uses

Buffers; Excipients

National Library of Medicine's Medical Subject Headings online file (MeSH, 1999)

from HSDB

/Tromethamine is indicated/ for the prevention and correction of metabolic acidosis. /Included in US product label/

Novak, K.M. (ed.). Drug Facts and Comparisons 59th Edition 2005. Wolters Kluwer Health. St. Louis, Missouri 2005., p. 130

from HSDB

Metabolic Acidosis Associated with Cardiac Bypass Surgery. Tromethamine solution has been found to be primarily beneficial in correcting metabolic acidosis which may occur during or immediately following cardiac bypass surgical procedures. /Included in US product label/

Medical Economics Co; Physicians Desk Reference: Generics 2nd ed p.3033 (1996)

from HSDB

Correction of Acidity of ACD Blood in Cardiac Bypass Surgery. It is well known that ACD blood is acidic and becomes more acidic on storage. Tromethamine effectively corrects this acidity. Tromethamine solution may be added directly to the blood used to prime the pump-oxygenator. When ACD blood is brought to a normal pH range the patient is spared an initial acid load. Additional tromethamine may be indicated during cardiac bypass surgery should metabolic acidosis appear. /Included in US product label/

Medical Economics Co; Physicians Desk Reference: Generics 2nd ed p.3033 (1996)

from HSDB

Metabolic Acidosis Associated with Cardiac Arrest. Acidosis is nearly always one of the consequences of cardiac arrest and, in some instances, may even be a causative factor in arrest. It is important therefore, that the correction of acidosis should be started promptly with other resuscitative efforts. By correcting acidosis, tromethamine solution has caused the arrested heart to respond to resuscitative efforts after standard methods alone had failed. In these cases, tromethamine was given intraventricularly. It is to be noted, however, that such precariously ill patients often have died subsequently of causes unrelated to the administration of tromethamine. With administration by the peripheral venous route, metabolic acidosis has been corrected in a majority of patients. The success in reinstitution of cardiac rhythm by this means probably has not been of the same order of magnitude as with the intraventricular route. /Included in US product label/

Medical Economics Co; Physicians Desk Reference: Generics 2nd ed p.3033 (1996)

from HSDB

VET: As amine pH buffer to correct metabolic and respiratory acidosis /as well as/ in **salicylate** and **carbon dioxide** poisonings.

Rossoff, I.S. Handbook of Veterinary Drugs. New York: Springer Publishing Company, 1974., p. 624

from HSDB

7.6 Drug Warnings

Local reactions associated with administration of tromethamine may include local irritation and tissue inflammation or infection at the site of injection, a febrile response, chemical phlebitis, venospasm, hypervolemia, and iv thrombosis. The drug should be administered through a large needle or indwelling catheter to minimize venous irritation by the highly alkaline tromethamine solution. Extravasation may result in inflammation, necrosis, and sloughing of overlying skin. If perivascular infiltration occurs, tromethamine administration should be discontinued immediately. Infiltration of the affected area with 1% **procaine hydrochloride**, to which hyaluronidase has been added, will often reduce venospasm and also will dilute any tromethamine remaining in the tissues locally. Local infiltration of an alpha-adrenergic blocking agent, such as **phentolamine mesylate**, into the vasospastic area has been recommended. If necessary, nerve block of autonomic fibers to the affected area may be performed.

McEvoy, G.K. (ed.). American Hospital Formulary Service. AHFS Drug Information. American Society of Health-System Pharmacists, Bethesda, MD. 2007., p. 2647

▸ **from HSDB**

Transient decreases in blood **glucose** concentration may occur during administration of tromethamine. When larger than recommended doses are used or when administration is too rapid, hypoglycemia may persist for several hours after the drug is discontinued.

McEvoy, G.K. (ed.). American Hospital Formulary Service. AHFS Drug Information. American Society of Health-System Pharmacists, Bethesda, MD. 2007., p. 2647

▸ **from HSDB**

Tromethamine should be slowly administered and in amounts sufficient only to correct the existing acidosis, in order to avoid overdosage and alkalosis. Determinations of blood **glucose** concentrations should be frequently performed during and following therapy.

McEvoy, G.K. (ed.). American Hospital Formulary Service. AHFS Drug Information. American Society of Health-System Pharmacists, Bethesda, MD. 2007., p. 2647

▸ **from HSDB**

Respiratory depression may occur in patients receiving large doses of tromethamine, as a result of increased blood pH and reduced carbon dioxide concentrations, and in those with chronic hypoventilation or those receiving other drugs that depress respiration. Dosage must be carefully adjusted so that blood pH does not increase above normal, and facilities for providing mechanical ventilation should be readily available during administration of tromethamine. Tromethamine may be used in conjunction with mechanical ventilatory support if respiratory acidosis is present concomitantly with metabolic acidosis.

McEvoy, G.K. (ed.). American Hospital Formulary Service. AHFS Drug Information. American Society of Health-System Pharmacists, Bethesda, MD. 2007., p. 2647

▸ **from HSDB**

Determinations of blood pH, **carbon dioxide** tension, and **bicarbonate**, **glucose**, and electrolyte concentrations should be performed before, during, and following administration of tromethamine. Tromethamine solutions should not be prepared extemporaneously in a concentration exceeding 0.3 M. Hemorrhagic necrosis of the liver has occurred in a number of seriously ill neonates who received hypertonic (1.2 M) preparations of tromethamine via the umbilical vein. Administration of a hypertonic solution (1.5 M) of tromethamine to adult patients has been reported to produce hydropic degeneration of hepatic and renal tubular cells.

McEvoy, G.K. (ed.). American Hospital Formulary Service. AHFS Drug Information. American Society of Health-System Pharmacists, Bethesda, MD. 2007., p. 2647

▸ **from HSDB**

Tromethamine has caused increased blood coagulation time in dogs and the possibility of such an occurrence in humans should be considered.

McEvoy, G.K. (ed.). American Hospital Formulary Service. AHFS Drug Information. American Society of Health-System Pharmacists, Bethesda, MD. 2007., p. 2647

▸ **from HSDB**

Tromethamine may produce hyperkalemia in patients with decreased renal function; ECG monitoring and frequent serum **potassium** determinations should be performed in such patients during therapy with the drug. Since tromethamine may accumulate in patients with decreased renal function, extreme caution is necessary if the drug is administered to patients with renal disease; the drug is contraindicated in patients with anuria or uremia. Except in life-threatening situations, tromethamine should not be administered for longer than 1 day; clinical experience has been generally limited to short-term use.

McEvoy, G.K. (ed.). American Hospital Formulary Service. AHFS Drug Information. American Society of Health-System Pharmacists, Bethesda, MD. 2007., p. 2647

▸ **from HSDB**

The safety and efficacy of tromethamine in pediatric patients is based on extensive (over 30 years) clinical experience documented in the medical literature and by safety surveillance. Tromethamine has been used in the treatment of severe cases of metabolic acidosis with concurrent respiratory acidosis in neonates and infants with respiratory failure, because unlike **sodium bicarbonate**, tromethamine does not elevate **carbon dioxide** tension (PaCO2). The drug also has been used in neonates and infants with hypernatremia and metabolic acidosis to avoid the additional **sodium** given with the **bicarbonate**. However, because the osmotic effects of tromethamine are greater and large continuous doses of the drug are required, **sodium bicarbonate** is preferred to tromethamine in the treatment of acidosis in neonates and infants with respiratory distress syndrome (RDS).

McEvoy, G.K. (ed.). American Hospital Formulary Service. AHFS Drug Information. American Society of Health-System Pharmacists, Bethesda, MD. 2007., p. 2647

▸ from HSDB

Intravenous infusions of tromethamine via low-lying umbilical venous catheters have been associated with occurrences of hepatocellular necrosis. In addition, hypoglycemia may occur when tromethamine is used in premature and even in full-term neonates.

McEvoy, G.K. (ed.). American Hospital Formulary Service. AHFS Drug Information. American Society of Health-System Pharmacists, Bethesda, MD. 2007., p. 2647

▸ from HSDB

Tromethamine is contraindicated in neonates with chronic respiratory acidosis and **salicylate** intoxication.

McEvoy, G.K. (ed.). American Hospital Formulary Service. AHFS Drug Information. American Society of Health-System Pharmacists, Bethesda, MD. 2007., p. 2647

▸ from HSDB

Tromethamine is contraindicated in uremia and anuria.

Medical Economics Co; Physicians Desk Reference: Generics 2nd ed p.3033 (1996)

▸ from HSDB

... Because geriatric patients may have decreased renal function and because patients with renal impairment may be at increased risk of tromethamine-induced toxicity, patients in this age group should have renal function monitored and dosage adjusted accordingly.

McEvoy, G.K. (ed.). American Hospital Formulary Service. AHFS Drug Information. American Society of Health-System Pharmacists, Bethesda, MD. 2007.

▸ from HSDB

It is not known whether tromethamine is distributed in human milk. Because many drugs are distributed into milk, the manufacturer recommends that the drug be used with caution in nursing women.

McEvoy, G.K. (ed.). American Hospital Formulary Service. AHFS Drug Information. American Society of Health-System Pharmacists, Bethesda, MD. 2007., p. 2647

▸ from HSDB

Because clinical experience has been limited generally to short-term use, the drug should not be administered for more than a period of one day except in a life-threatening situation.

Medical Economics Co; Physicians Desk Reference: Generics 2nd ed p.3033 (1996)

▸ from HSDB

FDA Pregnancy Risk Category: C /RISK CANNOT BE RULED OUT. Adequate, well controlled human studies are lacking, and animal studies have shown risk to the fetus or are lacking as well. There is a chance of fetal harm if the drug is given during pregnancy; but the potential benefits may outweigh the potential risk./

Medical Economics Co; Physicians Desk Reference: Generics 2nd ed p.3033 (1996)

▸ from HSDB

Additives may be incompatible. Consult with pharmacist, if available. When introducing additives, use aseptic technique, mix thoroughly and do not store.

Medical Economics Co; Physicians Desk Reference: Generics 2nd ed p.3033 (1996)

▸ from HSDB

Do not administer /tromethamine/ unless solution is clear and seal is intact.

Medical Economics Co; Physicians Desk Reference: Generics 2nd ed p.3033 (1996)

▸ from HSDB

Fact that about 70% remains in extracellular space means that sufficient amounts of **water** must be given to prevent hyperosmolarity and hence to avoid tissue dehydration and hemodynamic consequences of increased blood volume.

Osol, A. and J.E. Hoover, et al. (eds.). Remington's Pharmaceutical Sciences. 15th ed. Easton, Pennsylvania: Mack Publishing Co., 1975., p. 773

▸ from HSDB

7.7 Reported Fatal Dose

3. 3= MODERATELY TOXIC: PROBABLY ORAL LETHAL DOSE (HUMAN) 0.5-5 G/KG, BETWEEN 1 OZ & 1 PINT FOR 70 KG PERSON (150 LB).

Gosselin, R.E., H.C. Hodge, R.P. Smith, and M.N. Gleason. Clinical Toxicology of Commercial Products. 4th ed. Baltimore: Williams and Wilkins, 1976., p. II-74

▸ from HSDB

8 Pharmacology and Biochemistry

8.1 MeSH Pharmacological Classification

Buffers

A chemical system that functions to control the levels of specific ions in solution. When the level of hydrogen ion in solution is controlled the system is called a pH buffer. (See **all compounds classified as Buffers**.)

▶ from MeSH

Excipients

Usually inert substances added to a prescription in order to provide suitable consistency to the dosage form. These include binders, matrix, base or diluent in pills, tablets, creams, salves, etc. (See **all compounds classified as Excipients**.)

▶ from MeSH

8.2 ATC Code

B - Blood and blood forming organs

B05 - Blood substitutes and perfusion solutions

B05B - I.v. solutions

B05BB - Solutions affecting the electrolyte balance

B05BB03 - Trometamol

▶ from WHO ATC

B - Blood and blood forming organs

B05 - Blood substitutes and perfusion solutions

B05X - I.v. solution additives

B05XX - Other i.v. solution additives

B05XX02 - Trometamol

▶ from WHO ATC

8.3 Absorption, Distribution and Excretion

Tromethamine is substantially eliminated by the kidneys. ... Ionized tromethamine (chiefly as the **bicarbonate** salt) is rapidly and preferentially excreted in urine at a rate that depends on the infusion rate. The manufacturer states that urinary excretion continues over a period of 3 days; 75% or more appears in the urine after 8 hours. In some studies, 50-75% of an iv dose was recovered in urine within 24 hours, but another study reported recovery in healthy adults to be 64% and 77% after 2 and 3 days, respectively.

McEvoy, G.K. (ed.). American Hospital Formulary Service. AHFS Drug Information. American Society of Health-System Pharmacists, Bethesda, MD. 2007., p. 2647

▶ **from HSDB**

It is not known whether tromethamine is distributed in human milk.

McEvoy, G.K. (ed.). American Hospital Formulary Service. AHFS Drug Information. American Society of Health-System Pharmacists, Bethesda, MD. 2007., p. 2647

▶ **from HSDB**

Ionized tromethamine is excreted by kidney, so the effect is that of excretion of **hydrogen** ions. Elimination of drug from body is entirely by renal excretion. Excretion of tromethamine is accompanied by osmotic diuresis, since clinical doses of drug considerably add to osmolarity of glomerular filtrate.

Osol, A. and J.E. Hoover, et al. (eds.). Remington's Pharmaceutical Sciences. 15th ed. Easton, Pennsylvania: Mack Publishing Co., 1975., p. 773

▶ **from HSDB**

In rats of different age (5 to 240 days old) the renal excretion of Trishydroxymethylaminomethane (THAM) was studied. In 5 and in 240 days old rats the renal excretion of THAM was slower than in rats of other age groups. Stimulation of diuresis by i.p. injection of **mannitol**, thiazide or by oral **water** load resulted in an increase in THAM excretion in 5 and in 240 days old rats. The renal excretion of THAM was also increased by repeated administration of THAM in all age groups, except in new born rats. Possible mechanisms of action are discussed.

Braunlich H; Arch Int Pharmacodyn Ther 216 (1): 144-59 (1975)

PMID:240333

▶ **from HSDB**

The distribution of 14C labelled THAM (tris-hydroxymethylaminomethane) was determined between intra- and extracellular space of nephrectomized Sprague-Dawley rats as a function of time at constant plasma pH of 7.4. The following results were obtained: An equilibrium in the distribution of THAM between ECS and ICS will not occur before 6-12 hours after administration. This indicates that THAM permeates very slowly into the intracellular compartment, which is in contrast to the general assumption that it quickly diffuses into the

intracellular space to restore the intracellular acidosis. THAM disappears from the extracellular space in a multiexponential fashion, indicating that it equilibrates with the different body tissues at largely variable rates. The equilibrium which occurs between both body compartments 6-12 hours after THAM application does not agree with the values which are expected for transfer of only the nonionised substance. At plasma pH 7.4 and a "mean whole body pHi" of 6.88, THAM is distributed with a distribution ratio of 4 (ICS/ECS), a value quite different from the value of 11 which would be expected for exclusive nonionic diffusion. Thus THAM is also transferred across the cell membrane in ionized form. These results indicate that the influx of THAM into the intracellular space is too slow (when compared to the renal elimination kinetics) to influence intracellular pH significantly by direct buffer action. Moreover, only a fraction of THAM enters the intracellular space in the nonionized form, thus reducing (to an even greater extent) the direct effect of THAM on the intracellular acid-base equilibrium.

Rothe KF, Heisler N; Anasth Intensivther Notfallmed 19 (1): 24-6 (1984)

PMID:6711774

▶ **from HSDB**

8.4 Metabolism/Metabolites

Tromethamine is not metabolized appreciably.

McEvoy, G.K. (ed.). American Hospital Formulary Service. AHFS Drug Information. American Society of Health-System Pharmacists, Bethesda, MD. 2007., p. 2647

▶ **from HSDB**

8.5 Mechanism of Action

Tromethamine is an alkalinizing agent which acts as a proton (**hydrogen ion**) acceptor. Tromethamine is a weak base; following IV injection, it attracts and combines with **hydrogen** ions and their associated acid anions and the resulting salts are excreted in urine. Tromethamine can combine with lactic, pyruvic, and other metabolic acids and with **carbonic acid**. ... At pH 7.4, approximately 70% of the tromethamine present in plasma is in the ionized (protonated) form; if pH is decreased from pH 7.4, the ionized fraction of the drug is increased. In contrast to the ionized fraction of tromethamine, which upon administration reacts only with acid in the extracellular fluids, the fraction of the dose which remains un-ionized at physiologic pH is thought to be capable of penetrating the cell membrane to combine with intracellular acid. Since administration of tromethamine reduces **hydrogen ion** concentration, there is a decrease in proton donor and an increase in proton acceptor concentrations in body buffers. In the **bicarbonate**:**carbonic acid** buffer, the concentration of dissolved **carbon dioxide** is decreased (at least until regulatory mechanisms compensate) and the concentration of **bicarbonate** is increased. The reduction of **carbon dioxide** tension removes a potent stimulus to breathing and may result in hypoventilation and hypoxia.

McEvoy, G.K. (ed.). American Hospital Formulary Service. AHFS Drug Information. American Society of Health-System Pharmacists, Bethesda, MD. 2007., p. 2647

from HSDB

Tromethamine ... acts as a weak, osmotic diuretic, increasing the flow of alkaline urine containing increased amounts of electrolytes.

McEvoy, G.K. (ed.). American Hospital Formulary Service. AHFS Drug Information. American Society of Health-System Pharmacists, Bethesda, MD. 2007., p. 2647

from HSDB

By removing protons from hydronium ions, ionization of **carbonic acid** is shifted so as to decrease pCO2 and to increase **bicarbonate**. Excess **bicarbonate** is then gradually excreted in kidney. /Tromethamine is an/ especially useful way to manage excessively high pCO2 in respiratory acidosis...

Osol, A. and J.E. Hoover, et al. (eds.). Remington's Pharmaceutical Sciences. 15th ed. Easton, Pennsylvania: Mack Publishing Co., 1975., p. 773

from HSDB

8.6 Human Metabolite Information

8.6.1 Metabolite Description

Description

Tromethamine, also known as trometamol or tham, belongs to the class of organic compounds known as 1, 2-aminoalcohols. These are organic compounds containing an alkyl chain with an amine group bound to the C1 atom and an alcohol group bound to the C2 atom. Tromethamine is a drug which is used for the prevention and correction of metabolic acidosis. Tromethamine exists as a solid, soluble (in **water**), and a very weakly acidic compound (based on its pKa). Tromethamine is also a parent compound for other transformation products, including but not limited to, **bis-tris**, **bis-tris propane**, and **N-tris(hydroxymethyl)methylglycine**.

from Human Metabolome Database (HMDB)

9 Use and Manufacturing

9.1 Use Classification

Household Products	Personal care

Categories	

▸ from NLM Household Products Database

9.2 Household Products

NLM Household Products and Categories

Revlon **Vitamin C** Absolutes, Daily Radiance Cream, SPF 15 [Personal care]

Revlon **Vitamin C** Absolutes, Oil Free Radiance Lotion, SPF 15 [Personal care]

... see the **complete list of household products**

▸ from NLM Household Products Database

9.3 Uses

EPA CPDat Chemical and Product Categories

▸ from EPA Chemical and Products Database (CPDat)

In the synthesis of surface-active agents, vulcanization accelerators, pharmaceuticals. As emulsifying agent for cosmetic creams and lotions, mineral oil and paraffin wax emulsions, leather dressings, textile specialties, polishes, cleaning compounds, so-called soluble oils. Absorbent for acidic gases. Biological buffer.

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 1678

▸ **from HSDB**

Therapeutic Category: Alkalinizing agent

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 1678

▸ **from HSDB**

MEDICATION

▸ **from HSDB**

MEDICATION (VET)

▸ **from HSDB**

9.3.1 Industry Uses

Intermediates

Laboratory chemicals

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

▸ **from EPA Chemicals under the TSCA**

9.3.2 Consumer Uses

Non-TSCA use

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

▸ **from EPA Chemicals under the TSCA**

9.4 Methods of Manufacturing

... Prepared by reduction of **tris(hydroxymethyl)nitromethane**.

Ullmann's Encyclopedia of Industrial Chemistry. 6th ed.Vol 1: Federal Republic of Germany: Wiley-VCH Verlag GmbH & Co. 2003 to Present, p. V23 122 (2003)

from HSDB

May be prepared by reducation or catalytic hydrogenation of the corresponding nitro compd. ... Preparation by by electrolytic reduction: McMillan, US patent 2485982 (1949 to Comm Solvents Corp)

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 1677

from HSDB

9.5 Formulations/Preparations

Tromethamine formulations: Parenteral injection 36 mg/mL (18 g) Tham, Hospira.

McEvoy, G.K. (ed.). American Hospital Formulary Service. AHFS Drug Information. American Society of Health-System Pharmacists, Bethesda, MD. 2007., p. 2647

from HSDB

TROMETHAMINE, NF (THAM), IS AVAIL AS 0.3 MOLAR SOLN ADJUSTED TO PH 8.6 WITH **ACETIC ACID**. IT IS ALSO SUPPLIED AS POWDER (THAM-E) TO BE DISSOLVED IN 1 L OF STERILE **WATER**. EACH L CONTAINS 300 MMOLES (36 G) OF TROMETHAMINE, 30 MMOLES OF **SODIUM CHLORIDE**, & 5 MMOLES OF **POTASSIUM CHLORIDE**.

Goodman, L.S., and A. Gilman. (eds.) The Pharmacological Basis of Therapeutics. 5th ed. New York: Macmillan Publishing Co., Inc., 1975., p. 775

from HSDB

9.6 U.S. Production

Production volumes for non-confidential chemicals reported under the Inventory Update Rule.

Year	Production Range (pounds)
1986	>1 million - 10 million
1990	>1 million - 10 million
1994	>1 million - 10 million
1998	>1 million - 10 million
2002	>1 million - 10 million

*US EPA; Non-confidential Production Volume Information Submitted by Companies for Chemicals Under the 1986-2002 Inventory Update Rule (IUR). 1,3-Propanediol, 2-amino-2-(hydroxymethyl)- (77-86-1). Available from, as of March 20, 2008: **http://www.epa.gov/oppt/iur/tools/data/2002-vol.html***

from HSDB

1,3-Propanediol, 2-amino-2-(hydroxymethyl)- is listed as a High Production Volume (HPV) chemical (65FR81686). Chemicals listed as HPV were produced in or imported into the U.S. in >1 million pounds in 1990 and/or 1994. The HPV list is based on the 1990 Inventory Update Rule. (IUR) (40 CFR part 710 subpart B; 51FR21438).

*EPA/Office of Pollution Prevention and Toxics; High Production Volume (HPV) Challenge Program. Available from the Database Query page at: **http://www.epa.gov/hpv/pubs/general/opptsrch.htm** on 1,3-Propanediol, 2-amino-2-(hydroxymethyl)- (77-86-1) as of March 20, 2008*

from HSDB

9.7 Manufacturers

ANGUS Chemical Co., 1500 East Lake Road, Buffalo Grove, IL 60089 (800) 447-4369; Production site: Sterlington, LA 71280

SRI Consulting. 2007 Directory of Chemical Producers United States. Menlo Park, CA 2007, p. 943

from HSDB

GFS Chemicals Inc., PO Box 245, Powell, OH 43065, (740) 881-5501; Production site: Columbus, OH 43222

SRI Consulting. 2007 Directory of Chemical Producers United States. Menlo Park, CA 2007, p. 943

from HSDB

9.8 General Manufacturing Information

Industry Processing Sectors

All other basic organic chemical manufacturing

Pharmaceutical and medicine manufacturing

Wholesale and retail trade

from EPA Chemicals under the TSCA

EPA TSCA Commercial Activity Status

1,3-Propanediol, 2-amino-2-(hydroxymethyl)-: ACTIVE

https://www.epa.gov/tsca-inventory

▸ from EPA Chemicals under the TSCA

10 Identification

10.1 Analytic Laboratory Methods

ELECTROPHORESIS.

Association of Official Analytical Chemists. Official Methods of Analysis. 10th ed. and supplements. Washington, DC: Association of Official Analytical Chemists, 1965. New editions through 13th ed. plus supplements, 1982., p. 13/300-18.090

▸ from HSDB

Analyte: tromethamine; matrix: chemical identification; procedure: infrared absorption spectrophotometry with comparison to standards

U.S. Pharmacopeia. The United States Pharmacopeia, USP 30/The National Formulary, NF 25; Rockville, MD: U.S. Pharmacopeial Convention, Inc., p.3429 (2007)

▸ from HSDB

Analyte: tromethamine; matrix: chemical identification; procedure: reaction with salicylaldehyde and glacial acetic acid produces a yellow color

U.S. Pharmacopeia. The United States Pharmacopeia, USP 30/The National Formulary, NF 25; Rockville, MD: U.S. Pharmacopeial Convention, Inc., p.3429 (2007)

▸ from HSDB

Analyte: tromethamine; matrix: chemical identification; procedure: reaction with ceric ammonium nitrate in nitric acid produces color change from light yellow to orange

U.S. Pharmacopeia. The United States Pharmacopeia, USP 30/The National Formulary, NF 25; Rockville, MD: U.S. Pharmacopeial Convention, Inc., p.3429 (2007)

▸ from HSDB

Analyte: tromethamine; matrix: chemical purity; procedure: dissolution in water; addition of bromocresol purple indicator; titration with hydrochloric acid to a yellow endpoint

U.S. Pharmacopeia. The United States Pharmacopeia, USP 30/The National Formulary, NF 25; Rockville, MD: U.S. Pharmacopeial Convention, Inc., p.3429 (2007)

from HSDB

Analyte: tromethamine; matrix: pharmaceutical preparation (solid for injection); procedure: infrared absorption spectrophotometry with comparison to standards (chemical identification)

U.S. Pharmacopeia. The United States Pharmacopeia, USP 30/The National Formulary, NF 25; Rockville, MD: U.S. Pharmacopeial Convention, Inc., p.3429 (2007)

from HSDB

Analyte: tromethamine; matrix: pharmaceutical preparation (solid for injection); procedure: dissolution in **water**; addition of **bromocresol purple** indicator; titration with **hydrochloric acid** to a yellow endpoint (chemical purity)

U.S. Pharmacopeia. The United States Pharmacopeia, USP 30/The National Formulary, NF 25; Rockville, MD: U.S. Pharmacopeial Convention, Inc., p.3429 (2007)

from HSDB

Analyte: tromethamine; matrix: pharmaceutical preparation (ophthalmic solution); procedure: capillary electrophoresis with ultraviolet detection at 215 nm; limit of detection: 2.5 ug/mL

McArdle FA, Meehan CJ; Analyst 123: 1757-1760 (1998). As cited in: Lunn G; HPLC and CE Methods for Pharmaceutical Analysis. CD-ROM. New York, NY: John Wiley & Sons (2000)

from HSDB

Analyte: tromethamine; matrix: pharmaceutical preparation; procedure: high-performance liquid chromatography with conductivity detection

Hall RE et al; J Chromatogr A 718: 305-308 (1995). As cited in: Lunn G; HPLC and CE Methods for Pharmaceutical Analysis. CD-ROM. New York, NY: John Wiley & Sons (2000)

from HSDB

10.2 Clinical Laboratory Methods

GC METHOD FOR QUANTITATIVE DETERMINATION OF TRIS(HYDROXYMETHYL)AMINOMETHANE IN PLASMA.

HULSHOFF A, HB KOSTENBAUDER; GC METHOD FOR QUANTITATIVE DETERMINATION OF TRIS(HYDROXYMETHYL)AMINOMETHANE IN PLASMA; J CHROMATOGR 145(1) 155 (1978)

from HSDB

Analyte: tromethamine; matrix: blood (plasma, dried), amniotic fluid, cerebrospinal fluid, urine; procedure: high-performance liquid chromatography with ultraviolet detection at 254 nm

Davey JF, Ersser RS; J Chromatogr 528: 9-23 (1990). As cited in: Lunn G; HPLC and CE Methods for Pharmaceutical Analysis. CD-ROM. New York, NY: John Wiley & Sons (2000)

from HSDB

Analyte: tromethamine; matrix: blood (plasma); procedure: high-performance liquid chromatography with ultraviolet detection at 237 nm; limit of detection: 282 ng/mL

Gumbhir K, Mason WD; J Chromatogr 583: 99-104 (1992). As cited in: Lunn G; HPLC and CE Methods for Pharmaceutical Analysis. CD-ROM. New York, NY: John Wiley & Sons (2000)

from HSDB

Analyte: tromethamine; matrix: blood (plasma), urine; procedure: high-performance liquid chromatography with fluorescence detection at 460 nm (excitation) and 532 nm (emission); limit of quantitation: 5 ug/mL (urine); 1 ug/mL (plasma)

Morris MJ, Hsieh JYK; J Chromatogr 622: 87-92 (1993). As cited in: Lunn G; HPLC and CE Methods for Pharmaceutical Analysis. CD-ROM. New York, NY: John Wiley & Sons (2000)

from HSDB

11 Safety and Hazards

11.1 Hazards Identification

11.1.1 GHS Classification

Pictogram(s)	 Irritant
Signal	**Warning**
GHS Hazard Statements	Aggregated GHS information provided by 794 companies from 22 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies. Reported as not meeting GHS hazard criteria by 182 of 794 companies. For more detailed information, please visit **ECHA C&L website**

	Of the 20 notification(s) provided by 612 of 794 companies with hazard statement code(s): H315 (99.84%): Causes skin irritation [**Warning** Skin corrosion/irritation] H319 (100%): Causes serious eye irritation [**Warning** Serious eye damage/eye irritation] H335 (84.97%): May cause respiratory irritation [**Warning** Specific target organ toxicity, single exposure; Respiratory tract irritation] Information may vary between notifications depending on impurities, additives, and other factors. The percentage value in parenthesis indicates the notified classification ratio from companies that provide hazard codes. Only hazard codes with percentage values above 10% are shown.
Precautionary Statement Codes	P261, P264, P271, P280, P302+P352, P304+P340, P305+P351+P338, P312, P321, P332+P313, P337+P313, P362, P403+P233, P405, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)

▸ from European Chemicals Agency (ECHA)

11.2 Accidental Release Measures

11.2.1 Disposal Methods

SRP: At the time of review, 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.

▸ from HSDB

11.3 Handling and Storage

11.3.1 Storage Conditions

Tromethamine injection should be stored at 20-25 deg C; freezing should be avoided. Unused portions of tromethamine solution should be discarded.

McEvoy, G.K. (ed.). American Hospital Formulary Service. AHFS Drug Information. American Society of Health-System Pharmacists, Bethesda, MD. 2007., p. 2647

▸ from HSDB

11.4 Regulatory Information

11.4.1 FDA Requirements

The Approved Drug Products with Therapeutic Equivalence Evaluations List identifies currently marketed prescription drug products, incl tromethamine, approved on the basis of safety and effectiveness by FDA under sections 505 of the Federal Food, Drug, and Cosmetic Act.

DHHS/FDA; Electronic Orange Book-Approved Drug Products with Therapeutic Equivalence Evaluations. Available from, as of March 15, 2005: ***http://www.fda.gov/cder/ob/***

▸ from HSDB

12 Toxicity

12.1 Toxicological Information

12.1.1 Acute Effects

▸ from ChemIDplus

12.1.2 Human Toxicity Excerpts

/HUMAN EXPOSURE STUDIES/ In studies of tromethamine administration in healthy individuals, the ventilatory rate remained constant, but a reduced tidal volume produced a decrease in minute ventilation and in **carbon dioxide** output; arterial **oxygen** saturation decreased by an average of about 5%.

McEvoy, G.K. (ed.). American Hospital Formulary Service. AHFS Drug Information. American Society of Health-System Pharmacists, Bethesda, MD. 2007., p. 2647

▸ **from HSDB**

/SIGNS AND SYMPTOMS/ Too rapid administration and/or excessive amounts of tromethamine may cause alkalosis, hypoglycemia, overhydration or solute overload.

Medical Economics Co; Physicians Desk Reference: Generics 2nd ed p.3033 (1996)

▸ **from HSDB**

12.1.3 Non-Human Toxicity Excerpts

/LABORATORY ANIMALS: Acute Exposure/ Even after neutralization, large oral doses in lab animals cause weakness, collapse, & coma (without convulsions). Injections of high doses in animals produce hypoglycemia, but concurrent administration of **glucose** does not prevent death.

Gosselin, R.E., H.C. Hodge, R.P. Smith, and M.N. Gleason. Clinical Toxicology of Commercial Products. 4th ed. Baltimore: Williams and Wilkins, 1976., p. II-74

▸ **from HSDB**

12.1.4 Non-Human Toxicity Values

LD50 Rat iv 2300 mg/kg

Medical Economics Co; Physicians Desk Reference: Generics 2nd ed p.3033 (1996)

▸ **from HSDB**

LD50 Rat oral 5900 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. 3436

▸ **from HSDB**

LD50 Mouse iv 3500 mg/kg

Medical Economics Co; Physicians Desk Reference: Generics 2nd ed p.3033 (1996)

from HSDB

12.2 Ecological Information

12.2.1 Environmental Fate/Exposure Summary

Tromethamine's production and use as an emulsifying agent, in the synthesis of surface-active agents and vulcanization accelerators may result in its release to the environment through various waste streams. If released to air, an estimated vapor pressure of 2.2X10-5 mm Hg at 25 deg C indicates that tromethamine is expected to exist in both the vapor and particulate phase in the ambient atmosphere. Vapor-phase tromethamine is degraded in the atmosphere by reaction with photochemically-produced **hydroxyl** radicals; the half-life for this reaction in air is estimated to be 11hours. Particulate-phase tromethamine is removed from the atmosphere by wet and dry deposition. Tromethamine does not contain chromophores that absorb at wavelengths >290 nm and therefore is not expected to be susceptible to direct photolysis by sunlight. If released to soil, an estimated Koc value of 1 indicates that tromethamine is expected to possess very high mobility in soil. The pKa of tromethamine is 8.07. Thus, this compound will partially exist in cation form in the environment and cations generally adsorb to organic **carbon** and clay more strongly than their neutral counterparts. As a result, tromethamine may have greater adsorption and less mobility than its estimated Koc value indicates. Volatilization from moist soil is not expected since cations do not volatilize and the estimated Henry's Law constant for the neutral species (free base) of tromethamine is 8.7X10-13 atm cu m/mol. Tromethamine is not expected to volatilize from dry soil surfaces based upon its estimated vapor pressure. Tromethamine yielded no **oxygen** uptake when incubated with pure cultures of different strains of bacteria, indicating biodegradation may be slow in the environment. If released to **water**, tromethamine is not expected to adsorb to suspended solids and sediment based upon the estimated Koc. However, based on the pKa of 8.07, it should exist partially as a cation under environmental conditions (pH 5-9). As a result, tromethamine may have greater adsorption to suspended to solids and sediment than its estimated Koc value indicates. Volatilization from **water** surfaces will not be an important fate process since cations do not volatilize and given the estimated Henry's Law constant for the neutral species. An estimated BCF of 3 suggests the potential for bioconcentration in aquatic organisms is low. Hydrolysis is not expected to be an important environmental fate process since this compound lacks functional groups that hydrolyze under environmental conditions. Occupational exposure to tromethamine may occur through inhalation and dermal contact with this compound at workplaces where tromethamine is produced or used. (SRC)

from HSDB

12.2.2 Artificial Pollution Sources

Tromethamine's production and use as an emulsifying agent, in the synthesis of surface-active agents and vulcanization accelerators(1) may result in its release to the environment through various waste streams(SRC).

(1) O'Neil MJ; Merck Index, 14th ed, Whitehouse Station, NJ Merck & Co. p 1677 (2006)

from HSDB

12.2.3 Environmental Fate

TERRESTRIAL FATE: Based on a classification scheme(1), an estimated Koc value of 1(SRC), determined from a structure estimation method(2), indicates that tromethamine is expected to have very high mobility in soil(SRC). However, tromethamine has a pKa of 8.07(3) and should exist partially as a cation under environmental conditions (pH 5-9)(SRC). As a result, tromethamine may have greater adsorption and less mobility than its estimated Koc value indicates since cations generally adsorb more strongly to soils containing organic carbon and clay than neutral species(4). Volatilization of tromethamine from moist soil surfaces is not expected to be an important fate process(SRC) since cations do not volatilize and the estimated Henry's Law constant for the neutral species is 8.7X10-13 atm-cu m/mole(SRC), using a fragment constant estimation method(5). Tromethamine is not expected to volatilize from dry soil surfaces(SRC) based upon an estimated vapor pressure of 2.2X10-5 mm Hg(SRC), determined from a fragment constant method(6).

(1) Swann RL et al; Res Rev 85: 17-28 (1983) (2) Meylan WM et al; Environ Sci Technol 26: 1560-67 (1992) (3) Perinn DD; Dissociation Constants of Organic Bases in Aqueous Solution. IUPAC Chem Data Ser: Suppl 1972. London, England: Buttersworth (1972) (4) Doucette WJ; pp. 141-188 in Handbook of Property Estimation Methods for Chemicals. Boethling RS, Mackay D, eds. Boca Raton, FL: Lewis Publ (2000) (5) Meylan WM, Howard PH; Environ Toxicol Chem 10: 1283-93 (1991) (6) Lyman WJ; p. 31 in Environmental Exposure From Chemicals Vol I, Neely WB, Blau GE, eds, Boca Raton, FL: CRC Press (1985)

from HSDB

AQUATIC FATE: Based on a classification scheme(1), an estimated Koc value of 1(SRC), determined from a structure estimation method(2), indicates that tromethamine is not expected to adsorb to suspended solids and sediment(SRC). However, tromethamine has a pKa of 8.07(3) and should exist partially as a cation under environmental conditions (pH 5-9)(SRC). As a result, tromethamine may have greater adsorption to suspended solids and sediment than its estimated Koc value indicates(SRC). Volatilization from water is not expected(4) since cations do not volatilize and the estimated Henry's Law constant for the neutral species (free base) of tromethamine is 8.7X10-13 atm cu m/mol(SRC), calculated using a fragment constant estimation method(5). According to a classification scheme(6), an estimated BCF of 3(SRC), from an estimated log Kow of -1.56(7) and a regression-derived equation(8), suggests the potential for bioconcentration in aquatic organisms is low(SRC).

(1) Swann RL et al; Res Rev 85: 17-28 (1983) (2) Meylan WM et al; Environ Sci Technol 26: 1560-67 (1992) (3) Perinn DD; Dissociation Constants of Organic Bases in Aqueous Solution. IUPAC Chem Data Ser: Suppl 1972. London, England: Buttersworth (1972) (4) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 4-9, 15-1 to 15-29 (1990) (5) Meylan WM, Howard PH; Environ Toxicol Chem 10: 1283-93 (1991)(6) Franke C et al; Chemosphere 29: 1501-14 (1994) (7) Meylan WM et al; Environ Toxicol Chem 18: 664-72 (1999) (8) Meylan WM et al; Environ Toxicol Chem 18: 664-72 (1999)

from HSDB

ATMOSPHERIC FATE: According to a model of gas/particle partitioning of semivolatile organic compounds in the atmosphere(1), tromethamine, which has a an estimated vapor pressure of 2.2X10-5 mm Hg at 25 deg C(SRC), determined from a fragment constant method(2), is expected to exist in both the vapor and particulate phases in the ambient atmosphere. Vapor-phase tromethamine is degraded in the atmosphere by reaction with photochemically-produced **hydroxyl** radicals(SRC); the half-life for this reaction in air is estimated to be 11 hours(SRC), calculated from its rate constant of 3.4X10-11 cu cm/molecule-sec at 25 deg C(SRC) that was derived using a structure estimation method(3). Particulate-phase tromethamine is removed from the atmosphere by wet and dry deposition(SRC). Tromethamine does not contain chromophores that absorb at wavelengths >290 nm and therefore is not expected to be susceptible to direct photolysis by sunlight(4).

(1) Bidleman T.F.; Environ Sci Technol 22: 361-367 (1988) (2) Lyman WJ; p. 31 in Environmental Exposure From Chemicals Vol I, Neely WB, Blau GE, eds, Boca Raton, FL: CRC Press (1985) (3) Meylan WM, Howard PH; Chemosphere 26: 2293-99 (1993) (4) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 8-12 (1990)

from HSDB

12.2.4 Environmental Biodegradation

Tromethamine yielded no **oxygen** uptake when incubated with pure cultures of different strains of bacteria(1), indicating biodegradation may be slow in the environment.

(1) Kersters K, Deley J; Biochim Biophysica Acta 71: 311-331 (1963)

from HSDB

12.2.5 Environmental Abiotic Degradation

The rate constant for the vapor-phase reaction of tromethamine with photochemically-produced **hydroxyl** radicals has been estimated as 3.4X10-11 cu cm/molecule-sec at 25 deg C(SRC), using a structure estimation method(1). This corresponds to an atmospheric half-life of about 11 hours(SRC) at an atmospheric concentration of 5X10+5 **hydroxyl** radicals per cu cm(1). Tromethamine is not expected to undergo hydrolysis in the environment due to the lack of hydrolyzable functional groups(2). Tromethamine does not contain chromophores that absorb at wavelengths >290 nm and therefore is not expected to undergo direct photolysis by sunlight(2).

(1) Meylan WM, Howard PH; Chemosphere 26: 2293-99 (1993) (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 7-4, 7-5, 8-12 (1990)

from HSDB

12.2.6 Environmental Bioconcentration

An estimated BCF of 3 was calculated for tromethamine (SRC), using an estimated log Kow of -1.56(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

(1) Meylan WM, Howard PH; J Pharm Sci 84: 83-92 (1995)(2) Meylan WM et al; Environ Toxicol Chem 18: 664-72 (1999) (3) Franke C et al; Chemosphere 29: 1501-14 (1994)

from HSDB

12.2.7 Soil Adsorption/Mobility

Using a structure estimation method based on molecular connectivity indices(1), the Koc of tromethamine can be estimated to be 1(SRC). According to a classification scheme(2), this estimated Koc value suggests that tromethamine is expected to have very high mobility in soil(SRC). The pKa of tromethamine is 8.07(3), indicating that this compound will partially exist as a cation in the environment. As a result, the mobility of tromethamine may be overestimated since cations generally adsorb more strongly to soils containing organic carbon and clay than neutral species(4).

(1) Meylan WM et al; Environ Sci Technol 26: 1560-67 (1992) (2) Swann RL et al; Res Rev 85: 17-28 (1983) (3) Perinn DD; Dissociation Constants of Organic Bases in Aqueous Solution. IUPAC Chem Data Ser: Suppl 1972. London, England: Buttersworth (1972) (4) Doucette WJ; pp. 141-188 in Handbook of Property Estimation Methods for Chemicals. Boethling RS, Mackay D, eds. Boca Raton, FL: Lewis Publ (2000)

from HSDB

12.2.8 Volatilization from Water/Soil

Tromethamine is a weak base with pKa of 8.07(1). This estimated pKa indicates tromethamine will partially exist in the protonated form in the environment. Volatilization from moist soil and water is not expected since cations do not volatilize and the estimated Henry's Law constant for the neutral species (free base) of tromethamine is 8.7X10-13 atm cu m/mol(SRC), using a fragment constant estimation method(2). Tromethamine is not expected to volatilize from dry soil surfaces(SRC) based upon an estimated vapor pressure of 2.2X10-5 mm Hg(SRC), determined from a fragment constant method(3).

(1) Perinn DD; Dissociation Constants of Organic Bases in Aqueous Solution. IUPAC Chem Data Ser: Suppl 1972. London, England: Buttersworth (1972) (2) Meylan WM, Howard PH; Environ Toxicol Chem 10: 1283-93 (1991) (3) Lyman WJ; p. 31 in Environmental Exposure From Chemicals Vol I, Neely WB, Blau GE, eds, Boca Raton, FL: CRC Press (1985)

from HSDB

12.2.9 Probable Routes of Human Exposure

NIOSH (NOES Survey 1981-1983) has statistically estimated that 40897 workers (30773 of these are female) are potentially exposed to tromethamine in the US(1). Occupational exposure to tromethamine may occur through inhalation and dermal contact with this compound at workplaces where tromethamine is produced or used(SRC).

(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 at ***http://www.cdc.gov/noes/*** *as of Dec 13, 2007.*

from HSDB

13 Literature

13.1 Depositor Provided PubMed Citations

from PubChem

13.2 NLM Curated PubMed Citations

from PubChem

13.3 Synthesis References

Jean Bourguignon, Marcel-Xavier Sion, Michel Moreau, "Preparation of tris(hydroxymethyl)aminomethane." U.S. Patent US4233245, issued August, 1959.

from DrugBank

13.4 Springer Nature References

from Springer Nature

13.5 Thieme References

from Thieme Chemistry

13.6 Chemical Co-Occurrences in Literature

from PubChem

13.7 Chemical-Disease Co-Occurrences in Literature

from PubChem

13.8 Chemical-Gene Co-Occurrences in Literature

from PubChem

14 Patents

14.1 Depositor-Supplied Patent Identifiers

from PubChem

15 Biomolecular Interactions and Pathways

15.1 Protein Bound 3-D Structures

View 1160 proteins in NCBI Structure

from PubChem

15.2 DrugBank Interactions

Showing 1 of 13 View More

Target	Autolysin
General Function	N-acetylmuramoyl-l-alanine amidase activity
Specific Function	Autolysins are involved in some important biological processes such as cell separation, cell-wall turnover, competence for genetic transformation, formation of the flagella and sporulation. Autolysin strictly depends on the presence of choline-containing cell walls for activity.
Interaction References	1. Overington JP, Al-Lazikani B, Hopkins AL: How many drug targets are there? Nat Rev Drug Discov. 2006 Dec;5(12):993-6. [PMID: 17139284] 2. Imming P, Sinning C, Meyer A: Drugs, their targets and the nature and number of drug targets. Nat Rev Drug Discov. 2006 Oct;5(10):821-34. [PMID: 17016423]

from DrugBank

16 Biological Test Results

16.1 BioAssay Results

from PubChem

17 Classification

17.1 Ontologies

17.1.1 MeSH Tree

from MeSH

17.1.2 ChEBI Ontology

from ChEBI

17.1.3 KEGG: ATC

from KEGG

17.1.4 KEGG: Additive

from KEGG

17.1.5 WHO ATC Classification System

from WHO ATC

17.1.6 WIPO IPC

from WIPO

17.1.7 ChemIDplus

from ChemIDplus

17.1.8 ChEMBL Target Tree

from ChEMBL

17.1.9 Household Products Database Tree

- from NLM Household Products Database

17.1.10 UN GHS Classification

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

17.1.11 EPA CPDat Classification

from EPA Chemical and Products Database (CPDat)

18 Information Sources

FILTER BY SOURCE ALL SOURCES

1. ChEBI

   Tris
   http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:9754

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

2. DrugBank

   Tromethamine
   http://www.drugbank.ca/drugs/DB03754
   http://www.drugbank.ca/drugs/DB03754#targets

3. Human Metabolome Database (HMDB)

   Tromethamine
   http://www.hmdb.ca/metabolites/HMDB0240288

4. ChemIDplus

   Tromethamine [USAN:USP]
   https://chem.nlm.nih.gov/chemidplus/sid/0000077861

   ChemIDplus Chemical Information Classification
   https://chem.sis.nlm.nih.gov/chemidplus/

5. DTP/NCI

   Trometamol
   https://dtp.cancer.gov/dtpstandard/servlet/dwindex?searchtype=NSC&outputformat=html&searchlist=65434

   Trometamol
   https://dtp.cancer.gov/dtpstandard/servlet/dwindex?searchtype=NSC&outputformat=html&searchlist=6365

6. EPA Chemicals under the TSCA

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

   1,3-Propanediol, 2-amino-2-(hydroxymethyl)-
   https://www.epa.gov/chemicals-under-tsca

7. ## EPA DSSTox

Tromethamine

https://comptox.epa.gov/dashboard/DTXSID2023723

8. ## European Chemicals Agency (ECHA)

> **LICENSE**
>
> Use of the information, documents and data from the ECHA website is subject to the terms and conditions of this Legal Notice, and subject to other binding limitations provided for under applicable law, the information, documents and data made available on the ECHA website may be reproduced, distributed and/or used, totally or in part, for non-commercial purposes provided that ECHA is acknowledged as the source: "Source: European Chemicals Agency, http://echa.europa.eu/". Such acknowledgement must be included in each copy of the material. ECHA permits and encourages organisations and individuals to create links to the ECHA website under the following cumulative conditions: Links can only be made to webpages that provide a link to the Legal Notice page.
>
> https://echa.europa.eu/web/guest/legal-notice

Trometamol

https://echa.europa.eu/substance-information/-/substanceinfo/100.000.969

Trometamol

https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/113562

9. ## ClinicalTrials.gov

> **LICENSE**
>
> The ClinicalTrials.gov data carry an international copyright outside the United States and its Territories or Possessions. Some ClinicalTrials.gov data may be subject to the copyright of third parties; you should consult these entities for any additional terms of use.
>
> https://clinicaltrials.gov/ct2/about-site/terms-conditions#Use

Tromethamine

https://clinicaltrials.gov/

10. ## DailyMed

TROMETHAMINE

https://dailymed.nlm.nih.gov/dailymed/search.cfm?labeltype=all&query=TROMETHAMINE

11. ## EPA Chemical and Products Database (CPDat)

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

trometamol

https://comptox.epa.gov/dashboard/DTXSID2023723#exposure

EPA CPDat Classification

https://www.epa.gov/chemical-research/chemical-and-products-database-cpdat

12. ## HSDB

TROMETHAMINE

https://toxnet.nlm.nih.gov/cgi-bin/sis/search/r?dbs+hsdb:@term+@rn+@rel+77-86-1

13. ## EU Clinical Trials Register

https://www.clinicaltrialsregister.eu/

14. ## FDA Orange Book
https://www.fda.gov/Drugs/InformationOnDrugs/ucm129662.htm

15. ## FDA/SPL Indexing Data
023C2WHX2V
https://www.fda.gov/ForIndustry/DataStandards/SubstanceRegistrationSystem-UniqueIngredientIdentifierUNII/

16. ## MassBank of North America (MoNA)
2-Amino-2-(hydroxymethyl)-1,3-propanediol
http://mona.fiehnlab.ucdavis.edu/spectra/browse?inchikey=LENZDBCJOHFCAS-UHFFFAOYSA-N

17. ## NMRShiftDB
https://pubchem.ncbi.nlm.nih.gov/substance/593487

18. ## NIST
Tris(hydroxymethyl)aminomethane
http://www.nist.gov/srd/nist1a.cfm

19. ## NIPH Clinical Trials Search of Japan
https://rctportal.niph.go.jp/en/

20. ## NLM Household Products Database
Tromethamine
https://hpd.nlm.nih.gov/cgi-bin/household/brands?tbl=chem&id=1069
Household Products Classification
https://hpd.nlm.nih.gov/

21. ## SpectraBase
https://spectrabase.com/spectrum/6NemRBIDHcf
https://spectrabase.com/spectrum/D87jrBc99AD
https://spectrabase.com/spectrum/DAVlacXwzxe
https://spectrabase.com/spectrum/4ZaLbsVGQg2
https://spectrabase.com/spectrum/CsEm9nId2Ns
https://spectrabase.com/spectrum/1ihmQpvYzEW
https://spectrabase.com/spectrum/EqEJiTfJUjp
https://spectrabase.com/spectrum/EwFoHTJJNzE

22. ## Springer Nature

23. ## The Cambridge Structural Database
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=128604
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=177995
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=186550
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=654657
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=654658
https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=654659

24. ## Thieme Chemistry

25. WHO ATC
https://www.whocc.no/atc/

ATC Code
https://www.whocc.no/atc_ddd_index/

26. Wikipedia

tromethamine
https://en.wikipedia.org/wiki/Tris

27. MeSH

Tromethamine
https://www.ncbi.nlm.nih.gov/mesh/68014325

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

Buffers
https://www.ncbi.nlm.nih.gov/mesh/68002021

Excipients
https://www.ncbi.nlm.nih.gov/mesh/68005079

28. PubChem
https://pubchem.ncbi.nlm.nih.gov

29. KEGG

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

Pharmaceutical additives in Japan
http://www.genome.jp/kegg-bin/get_htext?br08316.keg

30. WIPO

International Patent Classification
http://www.wipo.int/classifications/ipc/

31. 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

32. ChEMBL

Target Tree
https://www.ebi.ac.uk/chembl/target/browser

33. NCBI
https://www.ncbi.nlm.nih.gov/projects/linkout