2

*** CHEMICAL IDENTIFICATION ***

RTECS NUMBER : DH6910000
CHEMICAL NAME : Benzoic acid, thio-, S-ester with N-((4-amino-2-methyl-5-pyrimidinyl)methyl)-N-(4-hydroxy- 2-mercapto-1-methyl-1-butenyl)formamide dihydrogen phosphate (ester)
CAS REGISTRY NUMBER : 22457-89-2
BEILSTEIN REFERENCE NO. : 0771326
LAST UPDATED : 199612
DATA ITEMS CITED : 2
MOLECULAR FORMULA : C19-H23-N4-O6-P-S
MOLECULAR WEIGHT : 466.49
WISWESSER LINE NOTATION : T6N CNJ B1 DZ E1VMY1&UYSVR&2OPQQO
COMPOUND DESCRIPTOR : Drug
SYNONYMS/TRADE NAMES :

* Benfotiamine
* Benzoylthiamine monophosphate
* Benzoylthiamine O-monophosphate
* S-Benzoylthiamine monophosphate
* Berdi
* Betivina
* Bietamine
* Biotamin
* BTMP
* 8088 C.B.
* Neurostop
* Nitanevril
* Tabiomyl
* Thiamine monophosphate benzoyl
* Vitanevril

*** HEALTH HAZARD DATA ***

** ACUTE TOXICITY DATA **

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Oral
SPECIES OBSERVED : Rodent - mouse
DOSE/DURATION : 15 gm/kg
TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value
REFERENCE :
NIIRDN Drugs in Japan (Ethical Drugs). (Yakugyo Jiho Co., Ltd., Tokyo, Japan) Volume(issue)/page/year: 6,781,1982

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Intravenous
SPECIES OBSERVED : Rodent - mouse
DOSE/DURATION : 2200 mg/kg
TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value
REFERENCE :
85IPAE "Modern Pharmaceuticals of Japan, III," Tokyo, Japan Pharmaceutical, Medical and Dental Supply Exporters' Assoc., 1968 Volume(issue)/page/year: -,78,1968

*** END OF RECORD ***

*** CHEMICAL IDENTIFICATION ***

RTECS NUMBER : XI7350000
CHEMICAL NAME : Thiamine, chloride, hydrochloride
CAS REGISTRY NUMBER : 67-03-8
LAST UPDATED : 199701
DATA ITEMS CITED : 19
MOLECULAR FORMULA : C12-H17-N4-O-S.Cl-H.Cl
MOLECULAR WEIGHT : 337.30
WISWESSER LINE NOTATION : T6N CNJ B1 DZ E1- AT5K CSJ D2Q E1 &Q &G &GH
COMPOUND DESCRIPTOR : Drug
Human

SYNONYMS/TRADE NAMES :

* Aneurine hydrochloride
* Apate drops
* Beatine
* Bedome
* Begiolan
* Benerva
* Bequin
* Berin
* Betabion hydrochloride
* Betalin S
* Betaxin
* Bethiazine
* Beuion
* Bevitex
* Bevitine
* Bewon
* Biuno
* Bivatin
* Bivita
* Clotiamina
* Eskapen
* Eskaphen
* Lixa-Beta
* Metabolin
* Slowten
* THD
* Thiadoxine
* Thiaminal
* Thiamin chloride
* Thiamin dichloride
* Thiamine chloride
* Thiamine dichloride
* Thiamine hydrochloride
* Thiamin hydrochloride
* Thiaminium chloride hydrochloride
* Thiamol
* Thiavit
* Tiamidon
* Tiaminal
* Trophite
* USAF CB-20
* Vetalin S
* Vinothiam
* Vitamin B hydrochloride
* Vitamin B1 hydrochloride
* Vitamin B(sub 1) hydrochloride
* Vitaneuron

*** HEALTH HAZARD DATA ***

** ACUTE TOXICITY DATA **

TYPE OF TEST : LDLo - Lowest published lethal dose
ROUTE OF EXPOSURE : Intramuscular
SPECIES OBSERVED : Human - woman
DOSE/DURATION : 5 mg/kg
TOXIC EFFECTS :
Behavioral - coma
Vascular - BP lowering not characterized in autonomic section
Immunological Including Allergic - anaphylaxis
REFERENCE :
AJEMEN American Journal of Emergency Medicine. (WB Saunders, Philadelphia, PA) V.1- 1983- Volume(issue)/page/year: 13,371,1995

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Oral
SPECIES OBSERVED : Rodent - rat
DOSE/DURATION : 3710 mg/kg
TOXIC EFFECTS :
Peripheral Nerve and Sensation - spastic paralysis with or without sensory change
Behavioral - tremor
Lungs, Thorax, or Respiration - other changes
REFERENCE :
AGACBH Agents and Actions, A Swiss Journal of Pharmacology. (Birkhaeuser Verlag, POB 133, CH-4010 Basel, Switzerland) V.1- 1969/70- Volume(issue)/page/year: 4,125,1974

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Intraperitoneal
SPECIES OBSERVED : Rodent - rat
DOSE/DURATION : 481 mg/kg
TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value
REFERENCE :
FRPPAO Farmaco, Edizione Pratica. (Casella Postale 227, 27100 Pavia, Italy) V.8-43 1953-88 For publisher information, see FRMCE8 Volume(issue)/page/year: 24,712,1969

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Subcutaneous
SPECIES OBSERVED : Rodent - rat
DOSE/DURATION : 560 mg/kg
TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value
REFERENCE :
ARZNAD Arzneimittel-Forschung. Drug Research. (Editio Cantor Verlag, Postfach 1255, W-7960 Aulendorf, Fed. Rep. Ger.) V.1- 1951- Volume(issue)/page/year: 6,623,1956

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Intravenous
SPECIES OBSERVED : Rodent - rat
DOSE/DURATION : 118 mg/kg
TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value
REFERENCE :

AEPPAE Naunyn-Schmiedeberg's Archiv fuer Experimentelle Pathologie und Pharmakologie. (Berlin, Ger.) V.110-253, 1925-66. For publisher information, see NSAPCC. Volume(issue)/page/year: 236,149,1959

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Oral
SPECIES OBSERVED : Rodent - mouse
DOSE/DURATION : 8224 mg/kg
TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value
REFERENCE :
IZVIAK Internationale Zeitschrift fuer Vitaminforschung. International Review of Vitamin Research. (Bern, Switzerland) V.19-40, 1947-70. For publisher information, see IJVNAP. Volume(issue)/page/year: 37,82,1967

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Intraperitoneal
SPECIES OBSERVED : Rodent - mouse
DOSE/DURATION : 200 mg/kg
TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value
REFERENCE :
NTIS** National Technical Information Service. (Springfield, VA 22161) Formerly U.S. Clearinghouse for Scientific & Technical Information. Volume(issue)/page/year: AD277-689

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Intravenous
SPECIES OBSERVED : Rodent - mouse
DOSE/DURATION : 74 mg/kg
TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value
REFERENCE :
FRPPAO Farmaco, Edizione Pratica. (Casella Postale 227, 27100 Pavia, Italy) V.8-43 1953-88 For publisher information, see FRMCE8 Volume(issue)/page/year: 24,712,1969

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Intravenous
SPECIES OBSERVED : Mammal - cat
DOSE/DURATION : 75 mg/kg
TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value
REFERENCE :
ARZNAD Arzneimittel-Forschung. Drug Research. (Editio Cantor Verlag, Postfach 1255, W-7960 Aulendorf, Fed. Rep. Ger.) V.1- 1951- Volume(issue)/page/year: 6,623,1956

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Intravenous
SPECIES OBSERVED : Rodent - rabbit
DOSE/DURATION : 117 mg/kg
TOXIC EFFECTS :
Behavioral - muscle contraction or spasticity
Lungs, Thorax, or Respiration - cyanosis
Lungs, Thorax, or Respiration - other changes
REFERENCE :
PSEBAA Proceedings of the Society for Experimental Biology and Medicine. (Academic Press, Inc., 1 E. First St., Duluth, MN 55802) V.1- 1903/04- Volume(issue)/page/year: 68,153,1948

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Subcutaneous
SPECIES OBSERVED : Rodent - guinea pig
DOSE/DURATION : 872 mg/kg
TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value
REFERENCE :
ARZNAD Arzneimittel-Forschung. Drug Research. (Editio Cantor Verlag, Postfach 1255, W-7960 Aulendorf, Fed. Rep. Ger.) V.1- 1951-
Volume(issue)/page/year: 6,623,1956

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Intravenous
SPECIES OBSERVED : Rodent - guinea pig
DOSE/DURATION : 140 mg/kg
TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value
REFERENCE :
ARZNAD Arzneimittel-Forschung. Drug Research. (Editio Cantor Verlag, Postfach 1255, W-7960 Aulendorf, Fed. Rep. Ger.) V.1- 1951-
Volume(issue)/page/year: 6,623,1956

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Intravenous
SPECIES OBSERVED : Bird - pigeon
DOSE/DURATION : 180 mg/kg
TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value
REFERENCE :
ARZNAD Arzneimittel-Forschung. Drug Research. (Editio Cantor Verlag, Postfach 1255, W-7960 Aulendorf, Fed. Rep. Ger.) V.1- 1951-
Volume(issue)/page/year: 6,623,1956

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Subcutaneous
SPECIES OBSERVED : Amphibian - frog
DOSE/DURATION : 2600 mg/kg
TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value
REFERENCE :
ARZNAD Arzneimittel-Forschung. Drug Research. (Editio Cantor Verlag, Postfach 1255, W-7960 Aulendorf, Fed. Rep. Ger.) V.1- 1951-
Volume(issue)/page/year: 9,1,1959

** OTHER MULTIPLE DOSE TOXICITY DATA **

TYPE OF TEST : TDLo - Lowest published toxic dose
ROUTE OF EXPOSURE : Intraperitoneal
SPECIES OBSERVED : Rodent - rat
DOSE/DURATION : 8540 mg/kg/28D-I
TOXIC EFFECTS :
Related to Chronic Data - death
REFERENCE :
FRPPAO Farmaco, Edizione Pratica. (Casella Postale 227, 27100 Pavia, Italy) V.8-43 1953-88 For publisher information, see FRMCE8
Volume(issue)/page/year: 24,712,1969

TYPE OF TEST : TDLo - Lowest published toxic dose
ROUTE OF EXPOSURE : Subcutaneous

SPECIES OBSERVED : Rodent - mouse
DOSE/DURATION : 11200 mg/kg/28D-I
TOXIC EFFECTS :
Peripheral Nerve and Sensation - spastic paralysis with or without sensory change
Sense Organs and Special Senses (Eye) - effect, not otherwise specified
Behavioral - convulsions or effect on seizure threshold
REFERENCE :
ARZNAD Arzneimittel-Forschung. Drug Research. (Editio Cantor Verlag, Postfach 1255, W-7960 Aulendorf, Fed. Rep. Ger.) V.1- 1951-
Volume(issue)/page/year: 6,623,1956

*** NIOSH STANDARDS DEVELOPMENT AND SURVEILLANCE DATA ***

NIOSH OCCUPATIONAL EXPOSURE SURVEY DATA :
NOHS - National Occupational Hazard Survey (1974)
NOHS Hazard Code - 72200
No. of Facilities: 1288 (estimated)
No. of Industries: 6
No. of Occupations: 14
No. of Employees: 18364 (estimated)

NOES - National Occupational Exposure Survey (1983)
NOES Hazard Code - 72200
No. of Facilities: 1872 (estimated)
No. of Industries: 10
No. of Occupations: 28
No. of Employees: 48078 (estimated)
No. of Female Employees: 31774 (estimated)

*** STATUS IN U.S. ***

EPA TSCA Section 8(b) CHEMICAL INVENTORY

*** END OF RECORD ***

*** CHEMICAL IDENTIFICATION ***

RTECS NUMBER : QT0525000
CHEMICAL NAME : Nicotinic acid
CAS REGISTRY NUMBER : 59-67-6
BEILSTEIN REFERENCE NO. : 0109591
REFERENCE : 5-22-02-00057 (Beilstein Handbook Reference)
LAST UPDATED : 199710
DATA ITEMS CITED : 19
MOLECULAR FORMULA : C6-H5-N-O2
MOLECULAR WEIGHT : 123.12
WISWESSER LINE NOTATION : T6NJ CVQ
COMPOUND DESCRIPTOR : Tumorigen
Drug
Human

SYNONYMS/TRADE NAMES :

* Acide nicotinique
* Acidum nicotinicum
* Akotin
* Anti-pellagra vitamin
* Apelagrin
* Bionic
* 3-Carboxypyridine
* Daskil
* Davitamon PP
* Direktan
* Efacin
* Kyselina nikotinova
* NAH
* Naotin
* Niacin
* Nicacid
* Nicangin
* NICO
* Nico-400
* Nicobid
* Nicocap
* Nicocidin
* Nicocrisina
* Nicodan
* Nicodelmine
* Nicolar
* Niconacid
* Niconat
* Niconazid
* Nicosan 3
* Nicoside
* Nico-span
* Nicosyl
* Nicotamin
* Nicotene
* Nicotil
* Nicotine acid
* Nicotinipca
* Nicotinoylhydrazine
* Nicotinsaure
* Nicovasan
* Nicovasen
* Nicyl
* Nipellen

* Pellagramin
* Pellagra preventive factor
* Pellagrin
* Pelonin
* Peviton
* PP factor
* P.P. factor-pellagra preventive factor
* Pyridine-3-carbonic acid
* Pyridine-beta-carboxylic acid
* Pyridine-3-carboxylic acid
* 3-Pyridinecarboxylic acid
* Pyridine-carboxylique-3
* S115
* SK-Niacin
* SR 4390
* Tinic
* Vitaplex N
* Wampocap

*** HEALTH HAZARD DATA ***

** ACUTE TOXICITY DATA **

TYPE OF TEST : TDLo - Lowest published toxic dose
ROUTE OF EXPOSURE : Oral
SPECIES OBSERVED : Human - man
DOSE/DURATION : 2571 mg/kg/90D-I
TOXIC EFFECTS :
Blood - change in clotting factors
Blood - changes in platelet count
REFERENCE :
AIMDAP Archives of Internal Medicine. (AMA, 535 N. Dearborn St., Chicago, IL 60610) V.1- 1908- Volume(issue)/page/year: 152,861,1992

TYPE OF TEST : TDLo - Lowest published toxic dose
ROUTE OF EXPOSURE : Oral
SPECIES OBSERVED : Human - man
DOSE/DURATION : 9713 mg/kg/58W-I
TOXIC EFFECTS :
Gastrointestinal - nausea or vomiting
Skin and Appendages - sweating
Nutritional and Gross Metabolic - metabolic acidosis
REFERENCE :
SMJOAV Southern Medical Journal. (Southern Medical Assoc., POB 2446, Birmingham, AL 35205) V.1- 1908- Volume(issue)/page/year: 84,496,1991

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Oral
SPECIES OBSERVED : Rodent - rat
DOSE/DURATION : 7 gm/kg
TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value
REFERENCE :
NIIRDN Drugs in Japan (Ethical Drugs). (Yakugyo Jiho Co., Ltd., Tokyo, Japan) Volume(issue)/page/year: 6,544,1982

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Intraperitoneal
SPECIES OBSERVED : Rodent - rat
DOSE/DURATION : 730 mg/kg

TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value
REFERENCE :
OYYAA2 Oyo Yakuri. Pharmacometrics. (Oyo Yakuri Kenkyukai, CPO Box 180, Sendai 980-91, Japan) V.1- 1967- Volume(issue)/page/year: 14,741,1977

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Subcutaneous
SPECIES OBSERVED : Rodent - rat
DOSE/DURATION : 5 gm/kg
TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value
REFERENCE :
NIIRDN Drugs in Japan (Ethical Drugs). (Yakugyo Jiho Co., Ltd., Tokyo, Japan) Volume(issue)/page/year: 6,544,1982

TYPE OF TEST : LDLo - Lowest published lethal dose
ROUTE OF EXPOSURE : Intravenous
SPECIES OBSERVED : Rodent - rat
DOSE/DURATION : 3500 mg/kg
TOXIC EFFECTS :
Behavioral - convulsions or effect on seizure threshold
REFERENCE :
PSEBAA Proceedings of the Society for Experimental Biology and Medicine. (Academic Press, Inc., 1 E. First St., Duluth, MN 55802) V.1- 1903/04- Volume(issue)/page/year: 38,241,1938

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Oral
SPECIES OBSERVED : Rodent - mouse
DOSE/DURATION : 3720 mg/kg
TOXIC EFFECTS :
Behavioral - changes in motor activity (specific assay)
Lungs, Thorax, or Respiration - other changes
REFERENCE :
OYYAA2 Oyo Yakuri. Pharmacometrics. (Oyo Yakuri Kenkyukai, CPO Box 180, Sendai 980-91, Japan) V.1- 1967- Volume(issue)/page/year: 7,149,1973

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Intraperitoneal
SPECIES OBSERVED : Rodent - mouse
DOSE/DURATION : 358 mg/kg
TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value
REFERENCE :
OYYAA2 Oyo Yakuri. Pharmacometrics. (Oyo Yakuri Kenkyukai, CPO Box 180, Sendai 980-91, Japan) V.1- 1967- Volume(issue)/page/year: 14,741,1977

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Subcutaneous
SPECIES OBSERVED : Rodent - mouse
DOSE/DURATION : 3500 mg/kg
TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value
REFERENCE :
OYYAA2 Oyo Yakuri. Pharmacometrics. (Oyo Yakuri Kenkyukai, CPO Box 180, Sendai 980-91, Japan) V.1- 1967- Volume(issue)/page/year: 14,741,1977

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Intravenous

SPECIES OBSERVED : Rodent - mouse
DOSE/DURATION : 5 gm/kg
TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value
REFERENCE :
THERAP Therapie. (Doin, Editeurs, 8, Place de l'Odeon, F-75006 Paris, France) V.1- 1946- Volume(issue)/page/year: 26,831,1971

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Unreported
SPECIES OBSERVED : Rodent - mouse
DOSE/DURATION : 4 gm/kg
TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value
REFERENCE :
BAXXDU British UK Patent Application. (U.S. Patent and Trademark Office, Foreign Patents, Washington, DC 20231) Volume(issue)/page/year: #2041937

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Oral
SPECIES OBSERVED : Rodent - rabbit
DOSE/DURATION : 4550 mg/kg
TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value
REFERENCE :
OYYAA2 Oyo Yakuri. Pharmacometrics. (Oyo Yakuri Kenkyukai, CPO Box 180, Sendai 980-91, Japan) V.1- 1967- Volume(issue)/page/year: 14,741,1977

TYPE OF TEST : LDLo - Lowest published lethal dose
ROUTE OF EXPOSURE : Intravenous
SPECIES OBSERVED : Rodent - guinea pig
DOSE/DURATION : 3500 mg/kg
TOXIC EFFECTS :
Behavioral - convulsions or effect on seizure threshold
REFERENCE :
PSEBAA Proceedings of the Society for Experimental Biology and Medicine. (Academic Press, Inc., 1 E. First St., Duluth, MN 55802) V.1- 1903/04- Volume(issue)/page/year: 38,241,1938

** TUMORIGENIC DATA **

TYPE OF TEST : TDLo - Lowest published toxic dose
ROUTE OF EXPOSURE : Oral
SPECIES OBSERVED : Rodent - mouse
DOSE/DURATION : 174 gm/kg/94W-C
TOXIC EFFECTS :
Tumorigenic - Carcinogenic by RTECS criteria
Lungs, Thorax, or Respiration - tumors
REFERENCE :
ONCOBS Oncology. (S. Karger AG, Postfach CH-4009 Basel, Switzerland) V.21- 1967- Volume(issue)/page/year: 38,106,1981

*** OCCUPATIONAL EXPOSURE LIMITS ***

OEL-RUSSIA:STEL 1 mg/m3 JAN 1993

*** NIOSH STANDARDS DEVELOPMENT AND SURVEILLANCE DATA ***

NIOSH OCCUPATIONAL EXPOSURE SURVEY DATA :
NOHS - National Occupational Hazard Survey (1974)

NOHS Hazard Code - 81908
No. of Facilities: 1815 (estimated)
No. of Industries: 10
No. of Occupations: 19
No. of Employees: 13494 (estimated)

NOES - National Occupational Exposure Survey (1983)
NOES Hazard Code - 81908
No. of Facilities: 3028 (estimated)
No. of Industries: 15
No. of Occupations: 46
No. of Employees: 61057 (estimated)
No. of Female Employees: 26152 (estimated)

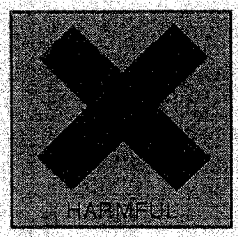
*** STATUS IN U.S. ***

EPA TSCA Section 8(b) CHEMICAL INVENTORY

EPA TSCA TEST SUBMISSION (TSCATS) DATA BASE, JUNE 1998

*** END OF RECORD ***

Safety (MSDS) data for adenine



General

Synonyms: adenine (synthetic), ADE, adeninimine, 6-aminopurine, 6-amino-1H-purine, 6-amino-3H-purine, vitamin B4, USAF CB-18
Molecular formula: $C_5H_5N_5$

CAS No: 73-24-5
EC No: 200-796-1

Physical data

Appearance: white crystalline solid
Melting point:
Boiling point:
Vapour density:
Vapour pressure:
Density (g cm^{-3}):
Flash point:
Explosion limits:
Autoignition temperature:
Water solubility: slight

Stability

Stable. Moisture-sensitive. Incompatible with strong oxidizing agents.

Toxicology

Harmful if consumed in more than small amounts. May cause reproductive or developmental defects.

Toxicity data
(The meaning of any abbreviations which appear in this section is given here.)
ORL-RAT LD50 227 mg kg^{-1}
IPR-RAT LD50 198 mg kg^{-1}
ORL-MUS LD50 783 mg kg^{-1}
IPR-MUS LD50 100 mg kg^{-1}
IVN-MUS LD50 > 30 mg kg^{-1}

Risk phrases
(The meaning of any risk phrases which appear in this section is given here.)
R20 R21 R22

Transport information

Non-hazardous for air, sea and road freight.

Personal protection

Minimize contact.

Safety phrases
(The meaning of any safety phrases which appear in this section is given here.)
S36.

[Return to Physical & Theoretical Chemistry Lab. Safety home page.]

This information was last updated on August 19, 2003. We have tried to make it as accurate and useful as possible, but can take no responsibility for its use, misuse, or accuracy. We have not verified this information, and cannot guarantee that it is up-to-date.

*** CHEMICAL IDENTIFICATION ***

RTECS NUMBER : RU4375000
CHEMICAL NAME : Pantothenic acid, calcium salt (2:1), (+)-
CAS REGISTRY NUMBER : 137-08-6
LAST UPDATED : 199701
DATA ITEMS CITED : 11
MOLECULAR FORMULA : C18-H32-N2-O10.Ca
MOLECULAR WEIGHT : 476.60
WISWESSER LINE NOTATION : QV2MVYQX1&1&1Q &-CA-
COMPOUND DESCRIPTOR : Drug
SYNONYMS/TRADE NAMES :
* Calcium D(+)-N-(alpha,gamma-dihydroxy-beta,beta-dimethylbutyryl)-beta-alaninate
* Calcium panthothenate
* Calcium pantothenate
* Calcium d-pantothenate
* d-Calcium pantothenate
* Calpanate
* Dextro calcium pantothenate
* N-(2,4-Dihydroxy-3,3-dimethylbutyryl)-beta-alanine calcium
* Pancal
* Panthoject
* Pantholin
* Pantothenate calcium
* Pantothenic acid, calcium salt
* Pantothenic acid, calcium salt, (+)-
* (+)-Pantothenic acid calcium salt
* Vitamin B-5

*** HEALTH HAZARD DATA ***

** ACUTE TOXICITY DATA **

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Oral
SPECIES OBSERVED : Rodent - rat
DOSE/DURATION : >10 gm/kg
TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value
REFERENCE :
NIIRDN Drugs in Japan (Ethical Drugs). (Yakugyo Jiho Co., Ltd., Tokyo, Japan) Volume(issue)/page/year: 6,599,1982

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Intraperitoneal
SPECIES OBSERVED : Rodent - rat
DOSE/DURATION : 820 mg/kg
TOXIC EFFECTS :
Behavioral - somnolence (general depressed activity)
Lungs, Thorax, or Respiration - other changes
REFERENCE :
PSEBAA Proceedings of the Society for Experimental Biology and Medicine. (Academic Press, Inc., 1 E. First St., Duluth, MN 55802) V.1- 1903/04- Volume(issue)/page/year: 45,311,1940

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Subcutaneous
SPECIES OBSERVED : Rodent - rat
DOSE/DURATION : 3400 mg/kg

TOXIC EFFECTS :
Behavioral - somnolence (general depressed activity)
Lungs, Thorax, or Respiration - other changes
REFERENCE :
PSEBAA Proceedings of the Society for Experimental Biology and Medicine. (Academic Press, Inc., 1 E. First St., Duluth, MN 55802) V.1- 1903/04- Volume(issue)/page/year: 45,311,1940

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Intravenous
SPECIES OBSERVED : Rodent - rat
DOSE/DURATION : 830 mg/kg
TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value
REFERENCE :
NIIRDN Drugs in Japan (Ethical Drugs). (Yakugyo Jiho Co., Ltd., Tokyo, Japan) Volume(issue)/page/year: 6,599,1982

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Oral
SPECIES OBSERVED : Rodent - mouse
DOSE/DURATION : 10 gm/kg
TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value
REFERENCE :
NIIRDN Drugs in Japan (Ethical Drugs). (Yakugyo Jiho Co., Ltd., Tokyo, Japan) Volume(issue)/page/year: 6,599,1982

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Intraperitoneal
SPECIES OBSERVED : Rodent - mouse
DOSE/DURATION : 920 mg/kg
TOXIC EFFECTS :
Behavioral - somnolence (general depressed activity)
Lungs, Thorax, or Respiration - other changes
REFERENCE :
PSEBAA Proceedings of the Society for Experimental Biology and Medicine. (Academic Press, Inc., 1 E. First St., Duluth, MN 55802) V.1- 1903/04- Volume(issue)/page/year: 45,311,1940

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Subcutaneous
SPECIES OBSERVED : Rodent - mouse
DOSE/DURATION : 2700 mg/kg
TOXIC EFFECTS :
Behavioral - somnolence (general depressed activity)
Lungs, Thorax, or Respiration - other changes
REFERENCE :
PSEBAA Proceedings of the Society for Experimental Biology and Medicine. (Academic Press, Inc., 1 E. First St., Duluth, MN 55802) V.1- 1903/04- Volume(issue)/page/year: 45,311,1940

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Intravenous
SPECIES OBSERVED : Rodent - mouse
DOSE/DURATION : 910 mg/kg
TOXIC EFFECTS :
Behavioral - somnolence (general depressed activity)
Lungs, Thorax, or Respiration - other changes
REFERENCE :

PSEBAA Proceedings of the Society for Experimental Biology and Medicine.
(Academic Press, Inc., 1 E. First St., Duluth, MN 55802) V.1- 1903/04-
Volume(issue)/page/year: 45,311,1940

*** NIOSH STANDARDS DEVELOPMENT AND SURVEILLANCE DATA ***

NIOSH OCCUPATIONAL EXPOSURE SURVEY DATA :

NOHS - National Occupational Hazard Survey (1974)
NOHS Hazard Code - 83849
No. of Facilities: 398 (estimated)
No. of Industries: 7
No. of Occupations: 22
No. of Employees: 19095 (estimated)

NOES - National Occupational Exposure Survey (1983)
NOES Hazard Code - 83849
No. of Facilities: 1870 (estimated)
No. of Industries: 10
No. of Occupations: 35
No. of Employees: 29697 (estimated)
No. of Female Employees: 7601 (estimated)

*** STATUS IN U.S. ***

EPA TSCA Section 8(b) CHEMICAL INVENTORY

*** END OF RECORD ***

*** CHEMICAL IDENTIFICATION ***

RTECS NUMBER : UV1350000
CHEMICAL NAME : Pyridoxol, hydrochloride
CAS REGISTRY NUMBER : 58-56-0
LAST UPDATED : 199712
DATA ITEMS CITED : 24
MOLECULAR FORMULA : C8-H11-N-O3.Cl-H
MOLECULAR WEIGHT : 205.66
WISWESSER LINE NOTATION : T6NJ B1 CQ D1Q E1Q &GH
COMPOUND DESCRIPTOR : Drug
Mutagen
Reproductive Effector
Human

SYNONYMS/TRADE NAMES :
* Adermine hydrochloride
* Becilan
* Benadon
* Campoviton 6
* Hexabetalin
* Hexabione hydrochloride
* Hexavibex
* Hexermin
* Hexobion
* 3-Hydroxy-4,5-dimethylol-alpha-picoline hydrochloride
* 5-Hydroxy-6-methyl-3,4-pyridinedicarbinol hydrochloride
* 5-Hydroxy-6-methyl-3,4-pyridinedimethanol hydrochloride
* 2-Methyl-3-hydroxy-4,5-bis(hydroxymethyl)pyridine hydrochloride
* 3,4-Pyridinedimethanol, 5-hydroxy-6-methyl-, hydrochloride
* Pyridipca
* Pyridoxine, hydrochloride
* Pyridoxinium chloride
* Pyridoxinum hydrochloricum
* Vitamin B6 hydrochloride

*** HEALTH HAZARD DATA ***

** ACUTE TOXICITY DATA **

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Oral
SPECIES OBSERVED : Rodent - rat
DOSE/DURATION : 4 gm/kg
TOXIC EFFECTS :
Behavioral - convulsions or effect on seizure threshold
Behavioral - excitement
REFERENCE :
ARZNAD Arzneimittel-Forschung. Drug Research. (Editio Cantor Verlag, Postfach 1255, W-7960 Aulendorf, Fed. Rep. Ger.) V.1- 1951-
Volume(issue)/page/year: 11,922,1961

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Subcutaneous
SPECIES OBSERVED : Rodent - rat
DOSE/DURATION : 3 gm/kg
TOXIC EFFECTS :
Behavioral - convulsions or effect on seizure threshold
Behavioral - excitement
REFERENCE :
ARZNAD Arzneimittel-Forschung. Drug Research. (Editio Cantor Verlag,

Postfach 1255, W-7960 Aulendorf, Fed. Rep. Ger.) V.1- 1951-
Volume(issue)/page/year: 11,922,1961

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Intravenous
SPECIES OBSERVED : Rodent - rat
DOSE/DURATION : 530 mg/kg
TOXIC EFFECTS :
Behavioral - convulsions or effect on seizure threshold
Behavioral - excitement
REFERENCE :
ARZNAD Arzneimittel-Forschung. Drug Research. (Editio Cantor Verlag,
Postfach 1255, W-7960 Aulendorf, Fed. Rep. Ger.) V.1- 1951-
Volume(issue)/page/year: 11,922,1961

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Oral
SPECIES OBSERVED : Rodent - mouse
DOSE/DURATION : 5500 mg/kg
TOXIC EFFECTS :
Behavioral - convulsions or effect on seizure threshold
Lungs, Thorax, or Respiration - dyspnea
REFERENCE :
ARZNAD Arzneimittel-Forschung. Drug Research. (Editio Cantor Verlag,
Postfach 1255, W-7960 Aulendorf, Fed. Rep. Ger.) V.1- 1951-
Volume(issue)/page/year: 11,922,1961

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Subcutaneous
SPECIES OBSERVED : Rodent - mouse
DOSE/DURATION : 2450 mg/kg
TOXIC EFFECTS :
Behavioral - convulsions or effect on seizure threshold
Lungs, Thorax, or Respiration - dyspnea
REFERENCE :
ARZNAD Arzneimittel-Forschung. Drug Research. (Editio Cantor Verlag,
Postfach 1255, W-7960 Aulendorf, Fed. Rep. Ger.) V.1- 1951-
Volume(issue)/page/year: 11,922,1961

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Intravenous
SPECIES OBSERVED : Rodent - mouse
DOSE/DURATION : 660 mg/kg
TOXIC EFFECTS :
Behavioral - convulsions or effect on seizure threshold
Lungs, Thorax, or Respiration - dyspnea
REFERENCE :
ARZNAD Arzneimittel-Forschung. Drug Research. (Editio Cantor Verlag,
Postfach 1255, W-7960 Aulendorf, Fed. Rep. Ger.) V.1- 1951-
Volume(issue)/page/year: 11,922,1961

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Oral
SPECIES OBSERVED : Mammal - dog
DOSE/DURATION : >500 mg/kg
TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value
REFERENCE :
ARZNAD Arzneimittel-Forschung. Drug Research. (Editio Cantor Verlag,
Postfach 1255, W-7960 Aulendorf, Fed. Rep. Ger.) V.1- 1951-

Volume(issue)/page/year: 11,922,1961

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Oral
SPECIES OBSERVED : Mammal - cat
DOSE/DURATION : 1 gm/kg
TOXIC EFFECTS :
Behavioral - convulsions or effect on seizure threshold
Gastrointestinal - changes in structure or function of salivary glands
Gastrointestinal - hypermotility, diarrhea
REFERENCE :
ARZNAD Arzneimittel-Forschung. Drug Research. (Editio Cantor Verlag, Postfach 1255, W-7960 Aulendorf, Fed. Rep. Ger.) V.1- 1951-
Volume(issue)/page/year: 11,922,1961

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Intravenous
SPECIES OBSERVED : Mammal - cat
DOSE/DURATION : 560 mg/kg
TOXIC EFFECTS :
Behavioral - convulsions or effect on seizure threshold
Gastrointestinal - changes in structure or function of salivary glands
Gastrointestinal - hypermotility, diarrhea
REFERENCE :
ARZNAD Arzneimittel-Forschung. Drug Research. (Editio Cantor Verlag, Postfach 1255, W-7960 Aulendorf, Fed. Rep. Ger.) V.1- 1951-
Volume(issue)/page/year: 11,922,1961

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Intramuscular
SPECIES OBSERVED : Mammal - cat
DOSE/DURATION : 500 mg/kg
TOXIC EFFECTS :
Behavioral - convulsions or effect on seizure threshold
Gastrointestinal - changes in structure or function of salivary glands
Gastrointestinal - hypermotility, diarrhea
REFERENCE :
ARZNAD Arzneimittel-Forschung. Drug Research. (Editio Cantor Verlag, Postfach 1255, W-7960 Aulendorf, Fed. Rep. Ger.) V.1- 1951-
Volume(issue)/page/year: 11,922,1961

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Intravenous
SPECIES OBSERVED : Rodent - rabbit
DOSE/DURATION : 464 mg/kg
TOXIC EFFECTS :
Peripheral Nerve and Sensation - spastic paralysis with or without sensory change
Behavioral - convulsions or effect on seizure threshold
REFERENCE :
ARZNAD Arzneimittel-Forschung. Drug Research. (Editio Cantor Verlag, Postfach 1255, W-7960 Aulendorf, Fed. Rep. Ger.) V.1- 1951-
Volume(issue)/page/year: 11,922,1961

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Intravenous
SPECIES OBSERVED : Bird - pigeon
DOSE/DURATION : 145 mg/kg
TOXIC EFFECTS :
Behavioral - altered sleep time (including change in righting reflex)

Behavioral - convulsions or effect on seizure threshold
REFERENCE :
ARZNAD Arzneimittel-Forschung. Drug Research. (Editio Cantor Verlag, Postfach 1255, W-7960 Aulendorf, Fed. Rep. Ger.) V.1- 1951- Volume(issue)/page/year: 11,922,1961

** OTHER MULTIPLE DOSE TOXICITY DATA **

TYPE OF TEST : TDLo - Lowest published toxic dose
ROUTE OF EXPOSURE : Oral
SPECIES OBSERVED : Mammal - dog
DOSE/DURATION : 21400 mg/kg/15W-I
TOXIC EFFECTS :
Spinal Cord - demyelination
Behavioral - changes in motor activity (specific assay)
Behavioral - ataxia
REFERENCE :
TXAPA9 Toxicology and Applied Pharmacology. (Academic Press, Inc., 1 E. First St., Duluth, MN 55802) V.1- 1959- Volume(issue)/page/year: 44,323,1978

** REPRODUCTIVE DATA **

TYPE OF TEST : TDLo - Lowest published toxic dose
ROUTE OF EXPOSURE : Oral
SPECIES OBSERVED : Human - woman
DOSE : 2 mg/kg
SEX/DURATION : female 38 week(s) after conception
TOXIC EFFECTS :
Reproductive - Maternal Effects - postpartum
REFERENCE :
APSVAM Acta Paediatrica Scandinavica. (Almqvist & Wiksell International, POB 4627, S-11691 Stockholm, Sweden) V.54-80 1965-91 For publisher information, see APAEEL Volume(issue)/page/year: 72,525,1983

TYPE OF TEST : TDLo - Lowest published toxic dose
ROUTE OF EXPOSURE : Intramuscular
SPECIES OBSERVED : Human - woman
DOSE : 2 mg/kg
SEX/DURATION : female 38 week(s) after conception
TOXIC EFFECTS :
Reproductive - Maternal Effects - postpartum
REFERENCE :
APSVAM Acta Paediatrica Scandinavica. (Almqvist & Wiksell International, POB 4627, S-11691 Stockholm, Sweden) V.54-80 1965-91 For publisher information, see APAEEL Volume(issue)/page/year: 72,525,1983

TYPE OF TEST : TDLo - Lowest published toxic dose
ROUTE OF EXPOSURE : Oral
SPECIES OBSERVED : Rodent - rat
DOSE : 8040 ug/kg
SEX/DURATION : female 14 week(s) pre-mating - 12 day(s) post-birth
TOXIC EFFECTS :
Reproductive - Specific Developmental Abnormalities - Central Nervous System
Reproductive - Effects on Newborn - biochemical and metabolic
REFERENCE :
JONUAI Journal of Nutrition. (Subscription Dept., 9650 Rockville Pike, Bethesda, MD 20014) V.1- 1928- Volume(issue)/page/year: 104,111,1974

TYPE OF TEST : TDLo - Lowest published toxic dose

ROUTE OF EXPOSURE : Oral
SPECIES OBSERVED : Rodent - rat
DOSE : 4 gm/kg
SEX/DURATION : female 6-15 day(s) after conception
TOXIC EFFECTS :
Reproductive - Effects on Newborn - growth statistics (e.g.%, reduced weight gain)
REFERENCE :
TOLED5 Toxicology Letters. (Elsevier Science Pub. B.V., POB 211, 1000 AE Amsterdam, Netherlands) V.1- 1977- Volume(issue)/page/year: 39,159,1987

TYPE OF TEST : TDLo - Lowest published toxic dose
ROUTE OF EXPOSURE : Intraperitoneal
SPECIES OBSERVED : Rodent - rat
DOSE : 15 gm/kg
SEX/DURATION : male 2 week(s) pre-mating
TOXIC EFFECTS :
Reproductive - Paternal Effects - testes, epididymis, sperm duct
REFERENCE :
EXMPA6 Experimental and Molecular Pathology. (Academic Press, Inc., 1 E. First St., Duluth, MN 55802) V.1- 1962- Volume(issue)/page/year: 55,63,1991

TYPE OF TEST : TDLo - Lowest published toxic dose
ROUTE OF EXPOSURE : Intraperitoneal
SPECIES OBSERVED : Rodent - rat
DOSE : 7500 mg/kg
SEX/DURATION : male 6 week(s) pre-mating
TOXIC EFFECTS :
Reproductive - Paternal Effects - prostate, seminal vesicle, Cowper's gland, accessory glands
REFERENCE :
ARTODN Archives of Toxicology. (Springer-Verlag, Heidelberger Pl. 3, D-1000 Berlin 33, Fed. Rep. Ger.) V.32- 1974- Volume(issue)/page/year: 66,198,1992

TYPE OF TEST : TDLo - Lowest published toxic dose
ROUTE OF EXPOSURE : Intraperitoneal
SPECIES OBSERVED : Rodent - rat
DOSE : 15 gm/kg
SEX/DURATION : male 6 week(s) pre-mating
TOXIC EFFECTS :
Reproductive - Paternal Effects - spermatogenesis (incl. genetic material, sperm morphology, motility, and count)
REFERENCE :
ARTODN Archives of Toxicology. (Springer-Verlag, Heidelberger Pl. 3, D-1000 Berlin 33, Fed. Rep. Ger.) V.32- 1974- Volume(issue)/page/year: 66,198,1992

** MUTATION DATA **

TYPE OF TEST : Mutation in microorganisms
TEST SYSTEM : Bacteria - Salmonella typhimurium
DOSE/DURATION : 5 mg/plate
REFERENCE :
TRENAF Kenkyu Nenpo--Tokyo-toritsu Eisei Kenkyusho. Annual Report of Tokyo Metropolitan Research Laboratory of Public Health. (Tokyo-toritsu Eisei Kenkyusho, 24-1, 3-chome, Hyakunin-cho, Shin-juku-ku, Tokyo 160, Japan) V.1- 1949/50- Volume(issue)/page/year: 37,447,1986

TYPE OF TEST : Sister chromatid exchange
TEST SYSTEM : Human Lymphocyte
DOSE/DURATION : 2 mg/L
REFERENCE :
MUREAV Mutation Research. (Elsevier Science Pub. B.V., POB 211, 1000 AE Amsterdam, Netherlands) V.1- 1964- Volume(issue)/page/year: 124,175,1983

*** NIOSH STANDARDS DEVELOPMENT AND SURVEILLANCE DATA ***

NIOSH OCCUPATIONAL EXPOSURE SURVEY DATA :
NOES - National Occupational Exposure Survey (1983)
NOES Hazard Code - X3950
No. of Facilities: 1955 (estimated)
No. of Industries: 8
No. of Occupations: 39
No. of Employees: 57249 (estimated)
No. of Female Employees: 35753 (estimated)

*** STATUS IN U.S. ***

EPA TSCA Section 8(b) CHEMICAL INVENTORY

*** END OF RECORD ***

*** CHEMICAL IDENTIFICATION ***

RTECS NUMBER : LP5425000
CHEMICAL NAME : Folic acid
CAS REGISTRY NUMBER : 59-30-3
LAST UPDATED : 199806
DATA ITEMS CITED : 15
MOLECULAR FORMULA : C19-H19-N7-O6
MOLECULAR WEIGHT : 441.45
WISWESSER LINE NOTATION : T66 BN DN GN JNJ CZ EQ H1MR DVMYVQ2VQ
COMPOUND DESCRIPTOR : Drug
Mutagen
Reproductive Effector

SYNONYMS/TRADE NAMES :
* Acifolic
* Cytofol
* Folacid
* Folacin
* Folbal
* Folcidin
* Foliamin
* Folipac
* Folsan
* Folsaure
* Folvite
* Glutamic acid, N-(p-(((2-amino-4-hydroxy-6-pteridinyl)methyl)amino)benzoyl)-, L-
* Glutamic acid, pteroyl-, L-
* Incafolic
* Kyselina listova
* Liver Lactobacillus casei factor
* Mittafol
* NSC 3073
* 4-Pteridinol, 2-amino-6-((p-((1,3-dicarboxypropyl)carbamoyl)anilino)methyl)-
* Pteroylglutamic acid
* Pteroyl-L-glutamic acid
* Pteroylmonoglutamic acid
* Pteroyl-L-monoglutamic acid
* USAF CB-13
* Vitamin B11
* Vitamin Bc
* Vitamin M

*** HEALTH HAZARD DATA ***

** ACUTE TOXICITY DATA **

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Intravenous
SPECIES OBSERVED : Rodent - rat
DOSE/DURATION : 500 mg/kg
TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value
REFERENCE :
NIIRDN Drugs in Japan (Ethical Drugs). (Yakugyo Jiho Co., Ltd., Tokyo, Japan) Volume(issue)/page/year: -,1409,1995

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Oral

SPECIES OBSERVED : Rodent - mouse
DOSE/DURATION : 10 gm/kg
TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value
REFERENCE :
TXAPA9 Toxicology and Applied Pharmacology. (Academic Press, Inc., 1 E. First St., Duluth, MN 55802) V.1- 1959- Volume(issue)/page/year: 23,537,1972

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Intraperitoneal
SPECIES OBSERVED : Rodent - mouse
DOSE/DURATION : 85 mg/kg
TOXIC EFFECTS :
Behavioral - convulsions or effect on seizure threshold
Behavioral - muscle weakness
Behavioral - coma
REFERENCE :
EXPEAM Experientia. (Birkhaeuser Verlag, POB 133, CH-4010 Basel, Switzerland) V.1- 1945- Volume(issue)/page/year: 41,72,1985

TYPE OF TEST : LDLo - Lowest published lethal dose
ROUTE OF EXPOSURE : Subcutaneous
SPECIES OBSERVED : Rodent - mouse
DOSE/DURATION : 200 mg/kg
TOXIC EFFECTS :
Kidney, Ureter, Bladder - other changes
Blood - changes in spleen
REFERENCE :
PSEBAA Proceedings of the Society for Experimental Biology and Medicine. (Academic Press, Inc., 1 E. First St., Duluth, MN 55802) V.1- 1903/04- Volume(issue)/page/year: 71,544,1949

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Intravenous
SPECIES OBSERVED : Rodent - mouse
DOSE/DURATION : 282 mg/kg
TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value
REFERENCE :
TXAPA9 Toxicology and Applied Pharmacology. (Academic Press, Inc., 1 E. First St., Duluth, MN 55802) V.1- 1959- Volume(issue)/page/year: 23,537,1972

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Intravenous
SPECIES OBSERVED : Rodent - rabbit
DOSE/DURATION : 410 mg/kg
TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value
REFERENCE :
NIIRDN Drugs in Japan (Ethical Drugs). (Yakugyo Jiho Co., Ltd., Tokyo, Japan) Volume(issue)/page/year: -,1409,1995

TYPE OF TEST : LD50 - Lethal dose, 50 percent kill
ROUTE OF EXPOSURE : Intravenous
SPECIES OBSERVED : Rodent - guinea pig
DOSE/DURATION : 120 mg/kg
TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value

REFERENCE :
NIIRDN Drugs in Japan (Ethical Drugs). (Yakugyo Jiho Co., Ltd., Tokyo, Japan) Volume(issue)/page/year: -,1409,1995

** REPRODUCTIVE DATA **

TYPE OF TEST : TDLo - Lowest published toxic dose
ROUTE OF EXPOSURE : Parenteral
SPECIES OBSERVED : Rodent - rat
DOSE : 150 mg/kg
SEX/DURATION : female 10 day(s) after conception
TOXIC EFFECTS :
Reproductive - Effects on Embryo or Fetus - cytological changes (including somatic cell genetic material)
REFERENCE :
FEPRA7 Federation Proceedings, Federation of American Societies for Experimental Biology. (Bethesda, MD) V.1-46, 1942-87. Volume(issue)/page/year: 23,292,1964

** MUTATION DATA **

TYPE OF TEST : Unscheduled DNA synthesis
ROUTE OF EXPOSURE : Intraperitoneal
TEST SYSTEM : Rodent - rat
DOSE/DURATION : 150 mg/kg
REFERENCE :
CNREA8 Cancer Research. (Public Ledger Building, Suit 816, 6th & Chestnut Sts., Philadelphia, PA 19106) V.1- 1941- Volume(issue)/page/year: 29,136,1969

TYPE OF TEST : Cytogenetic analysis
TEST SYSTEM : Rodent - rat Lymphocyte
DOSE/DURATION : 10 ug/L
REFERENCE :
ICDBEO In Vitro Cellular and Developmental Biology. (Tissue Culture Assoc., 19110 Montgomery Village Ave., Suite 300, Gaithersburg, MD 20879) V.21-1985- Volume(issue)/page/year: 22,681,1986

TYPE OF TEST : Unscheduled DNA synthesis
ROUTE OF EXPOSURE : Subcutaneous
TEST SYSTEM : Rodent - mouse
DOSE/DURATION : 150 mg/kg
REFERENCE :
LIFSAK Life Sciences. (Pergamon Press Inc., Maxwell House, Fairview Park, Elmsford, NY 10523) V.1-8, 1962-69; V.14- 1974- Volume(issue)/page/year: 14,1541,1974

TYPE OF TEST : Unscheduled DNA synthesis
ROUTE OF EXPOSURE : Intraperitoneal
TEST SYSTEM : Rodent - mouse
DOSE/DURATION : 250 mg/kg
REFERENCE :
CNREA8 Cancer Research. (Public Ledger Building, Suit 816, 6th & Chestnut Sts., Philadelphia, PA 19106) V.1- 1941- Volume(issue)/page/year: 29,136,1969

*** NIOSH STANDARDS DEVELOPMENT AND SURVEILLANCE DATA ***

NIOSH OCCUPATIONAL EXPOSURE SURVEY DATA :
NOHS - National Occupational Hazard Survey (1974)

NOHS Hazard Code - M1051
No. of Facilities: 220 (estimated)
No. of Industries: 4
No. of Occupations: 14
No. of Employees: 11106 (estimated)

NOES - National Occupational Exposure Survey (1983)
NOES Hazard Code - M1051
No. of Facilities: 2823 (estimated)
No. of Industries: 11
No. of Occupations: 40
No. of Employees: 60281 (estimated)
No. of Female Employees: 29903 (estimated)

*** STATUS IN U.S. ***

EPA TSCA Section 8(b) CHEMICAL INVENTORY

*** END OF RECORD ***

*** CHEMICAL IDENTIFICATION ***

RTECS NUMBER : GG3750000
CHEMICAL NAME : Cobinamide, cyanide phosphate 3'-ester with 5,6-dimethyl-1-alpha-D- ribofuranosylbenzimidazole, inner salt
CAS REGISTRY NUMBER : 68-19-9
BEILSTEIN REFERENCE NO. : 4122889
LAST UPDATED : 199706
DATA ITEMS CITED : 11
MOLECULAR FORMULA : C63-H88-Co-N14-O14-P
MOLECULAR WEIGHT : 1355.55
WISWESSER LINE NOTATION : D C5656 B-5 B6 B5 S5 J&5 B-19- Q&6 N&5/B-N/DU/J&-M& J&- O& 9ABBBBCSTT V& AN-CO-&& B-N CN TN C
COMPOUND DESCRIPTOR : Drug
Mutagen
Reproductive Effector

SYNONYMS/TRADE NAMES :

* Anacobin
* Berubigen
* Betalin-12
* Betalin 12 crystalline
* Betaline-12
* B-Twelve
* B-Twelve ora
* Byladoce
* Cabadon M
* CN-B12
* Cobadoce forte
* Cobalin
* Cobamin
* Cobione
* Cotel
* Covit
* Crystamin
* Crystwel
* Cyano-B12
* Cyanocobalamin
* Cyanocobalamine
* Cycolamin
* Cykobeminet
* Cyredin
* Cytacon
* Cytamen
* Cytobion
* Depinar
* Dimethylbenzimidazoylcobamide
* 5,6-Dimethylbenzimidazolylcobamide cyanide
* Distivit (B12 peptide)
* Dobetin
* Docemine
* Docibin
* Docigram
* Dodecabee
* Dodecavite
* Dodex
* Ducobee
* Duodecibin
* Embiol
* Emociclina

* Eritrone
* Erycytol
* Erythrotin
* Euhaemon
* Extrinsic factor
* Factor II
* Factor II (vitamin)
* Fresmin
* Hemo-B-doze
* Hemomin
* Hepagon
* Hepavis
* Hepcovite
* Lactobacillus lactis dorner factor
* LLD factor
* Macrabin
* Megalovel
* Milbedoce
* Nagravon
* Normocytin
* Pernaemon
* Pernaevit
* Pernipuron
* Plecyamin
* Poyamin
* Rebramin
* Redamina
* Redisol
* Rhodacryst
* Rubesol
* Rubramin
* Rubramin PC
* Rubripca
* Rubrocitol
* Sytobex
* Vibalt
* Vibisone
* Virubra
* Vitamin B12
* Vitamin B12 complex
* Vitamin B12 preparation
* Vitarubin
* Vita-rubra
* Vitral

*** HEALTH HAZARD DATA ***

** ACUTE TOXICITY DATA **

TYPE OF TEST : LD - Lethal dose
ROUTE OF EXPOSURE : Oral
SPECIES OBSERVED : Rodent - mouse
DOSE/DURATION : >5 gm/kg
TOXIC EFFECTS :
Details of toxic effects not reported other than lethal dose value
REFERENCE :
ARZNAD Arzneimittel-Forschung. Drug Research. (Editio Cantor Verlag, Postfach 1255, W-7960 Aulendorf, Fed. Rep. Ger.) V.1- 1951-
Volume(issue)/page/year: 42,114,1992

TYPE OF TEST : LDLo - Lowest published lethal dose
ROUTE OF EXPOSURE : Intraperitoneal
SPECIES OBSERVED : Rodent - mouse
DOSE/DURATION : 1364 ug/kg
TOXIC EFFECTS :
Behavioral - convulsions or effect on seizure threshold
Behavioral - excitement
REFERENCE :
ARPAAQ Archives of Pathology. (Chicago, IL) V.5(3)-50(3), 1928-50; V.70-99, 1960-75. For publisher information, see APLMAS.
Volume(issue)/page/year: 49,278,1950

TYPE OF TEST : LDLo - Lowest published lethal dose
ROUTE OF EXPOSURE : Subcutaneous
SPECIES OBSERVED : Rodent - mouse
DOSE/DURATION : 2727 ug/kg
TOXIC EFFECTS :
Lungs, Thorax, or Respiration - chronic pulmonary edema
Blood - other changes
REFERENCE :
ARPAAQ Archives of Pathology. (Chicago, IL) V.5(3)-50(3), 1928-50; V.70-99, 1960-75. For publisher information, see APLMAS.
Volume(issue)/page/year: 49,278,1950

** REPRODUCTIVE DATA **

TYPE OF TEST : TDLo - Lowest published toxic dose
ROUTE OF EXPOSURE : Oral
SPECIES OBSERVED : Rodent - rat
DOSE : 115 mg/kg
SEX/DURATION : female 1-22 day(s) after conception
TOXIC EFFECTS :
Reproductive - Effects on Newborn - growth statistics (e.g.%, reduced weight gain)
Reproductive - Effects on Newborn - biochemical and metabolic
REFERENCE :
NATUAS Nature. (Nature Subscription Dept., POB 1018, Manasguan, NJ 08736) V.1- 1869- Volume(issue)/page/year: 242,263,1973

TYPE OF TEST : TDLo - Lowest published toxic dose
ROUTE OF EXPOSURE : Intramuscular
SPECIES OBSERVED : Rodent - mouse
DOSE : 168 mg/kg
SEX/DURATION : female 10 day(s) after conception
TOXIC EFFECTS :
Reproductive - Specific Developmental Abnormalities - musculoskeletal system
Reproductive - Specific Developmental Abnormalities - urogenital system
REFERENCE :
JPMSAE Journal of Pharmaceutical Sciences. (American Pharmaceutical Assoc., 2215 Constitution Ave., NW, Washington, DC 20037) V.50- 1961-
Volume(issue)/page/year: 67,377,1978

TYPE OF TEST : TDLo - Lowest published toxic dose
ROUTE OF EXPOSURE : Intramuscular
SPECIES OBSERVED : Rodent - mouse
DOSE : 84 mg/kg
SEX/DURATION : female 11 day(s) after conception
TOXIC EFFECTS :
Reproductive - Effects on Embryo or Fetus - fetotoxicity (except death, e.g., stunted fetus)

REFERENCE :
JPMSAE Journal of Pharmaceutical Sciences. (American Pharmaceutical Assoc., 2215 Constitution Ave., NW, Washington, DC 20037) V.50- 1961-
Volume(issue)/page/year: 67,377,1978

*** NIOSH STANDARDS DEVELOPMENT AND SURVEILLANCE DATA ***

NIOSH RECOMMENDED EXPOSURE LEVEL (REL) :
NIOSH REL TO COBALT METAL, dust and fume-air:10H TWA 0.05 mg/m3
REFERENCE :
NIOSH* National Institute for Occupational Safety and Health, U.S. Dept. of Health, Education, and Welfare, Reports and Memoranda.
Volume(issue)/page/year: DHHS #92-100,1992

NIOSH OCCUPATIONAL EXPOSURE SURVEY DATA :
NOHS - National Occupational Hazard Survey (1974)
NOHS Hazard Code - 80358
No. of Facilities: 1219 (estimated)
No. of Industries: 6
No. of Occupations: 20
No. of Employees: 19601 (estimated)

NOES - National Occupational Exposure Survey (1983)
NOES Hazard Code - 80358
No. of Facilities: 3495 (estimated)
No. of Industries: 12
No. of Occupations: 46
No. of Employees: 65178 (estimated)
No. of Female Employees: 27980 (estimated)

*** STATUS IN U.S. ***

EPA GENETOX PROGRAM 1988, Inconclusive: Sperm morphology-human

EPA TSCA Section 8(b) CHEMICAL INVENTORY

*** END OF RECORD ***