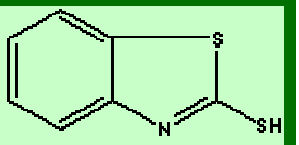
2-MERCAPTOBENZOTHIAZOLE



PRODUCT IDENTIFICATION

CAS NO.	149-30-4
EINECS NO.	205-736-8
FORMULA	$C_7H_5NS_2$
MOL WT.	167.24
H.S. CODE	2934.20.1500
TOXICITY	Oral, rat: LD50: 100 mg/kg
SYNONYMS	2-Benzothiazolethiol; captax; Rotax; Dermacid; MBT; Mercaptobenzothiazole; Mertax; Nocceler M; Thiotax; 2(3H)-Benzothiazolethione; Pennac MBT; Rokon; Sulfadene; Benzothiazolethiol; Bbenzothiazole-2-thiol; 2(3H)-Benzothiazolethione; Accelerator M; Vulkacit M; Vulkacit mercapto; Other RN: 1321-08-0; 4464-58-8; 12640-90-3; 55199-93-4; 81605-65-4; 112242-83-8; 119170-41-1
SMILES	c12c(sc(n1)S)cccc2
CLASSIFICATION	Anti-infective, Antifungal, Fungicide, Bactericide, Wood preservative, Rubber Chemical, Thiazole

PHYSICAL AND CHEMICAL PROPERTIES

PHYSICAL STATE	White to light yellow powder
MELTING POINT	171 C
BOILING POINT	260 C (Decomposes)
SPECIFIC GRAVITY	1.42
SOLUBILITY IN WATER	0.032 g/100ml
SOLVENT SOLUBILITY	Soluble in alkalies, alcohol, acetone, benzene and chloroform
VAPOR DENSITY	5.8
pKa	6.93 (Dissociation Constant at 20 C)
log Pow	2.42 (Octanol-water)
VAPOR PRESSURE	4.64E-04 (mmHg at 25 C)
HENRY'S LAW	3.63E-08 (atm-m3/mole at 25 C)
OH RATE	4.06E-11 (cm3/molecule-sec at 25 C Atmospheric)
AUTOIGNITION	465 C
REFRACTIVE INDEX	
NFPA RATINGS	Health: 2; Flammability: 0; Reactivity: 0
FLASH POINT	252 C
STABILITY	Stable under ordinary conditions

GENERAL DESCRIPTION & EXTERNAL LINKS

It is a moderately fast curing primary accelerator used in both dry rubber (natural and synthetic rubbers) and latex applications. Low temperature curing can be achieved in combination use with secondary accelerators, such as N,N'-diphenylguanidine, tetramethylthiuram disulfide, tetraethylthiuram disulfide. Vulcanizates obtained with MBT tend to have a relatively low modulus, but keep good aging properties. It is also used in latex foam curing systems. It is not recommended to be applied in rubber products connected with beverage and food due to bitter taste.

Related Salts: 155-04-4 (zinc salt), 2492-26-4 (hydrochloride salt), 26622-66-2 (mercury salt), 29904-98-1 (cobalt salt), 32510-27-3; 32510-27-3 (copper salt), 7778-70-3 (potassium salt)

2-Mercaptobenzothiazole, which is mainly used in the rubber industry as a vulcanization accelerator, is very toxic and is considered to be recalcitrant. We show here for the first time that it can be biotransformed and partially mineralized by a pure-culture bacterial strain of Rhodococcus rhodochrous. Three metabolites, among four detected, were identified. 2-Mercaptobenzothiazole (MBT) is the most important and most widely used member of the benzothiazole (BT) family. MBT is typically a rubber additive, but it has also other applications, such as inhibiting biocorrosion in cooling systems or in paper manufacturing. The annual MBT production in Western Europe is

estimated to be excess of 40,000 tons.

ASTM D7558 - 09 Standard Test Method for Colorimetric/Spectrophotometric Procedure to Quantify Extractable Chemical Dialkyldithiocarbamate, Thiuram, and Mercaptobenzothiazole Accelerators in Natural Rubber Latex and Nitrile Gloves

International Chemical Safety Cards

SALES SPECIFICATION	
APPEARANCE	White to light yellow powder
ASSAY (TITRATION)	96.0% min
MELTING POINT	171 C min
SIEVE ANALYSIS	0.5% max (+ 63 µm)
ASH	0.3% max
OIL CONTENT	0.2% max
LOSS ON DRYING	0.4% max

TRANSPORTATION	
PACKING	20kgs in Bag
HAZARD CLASS	6.1
UN NO.	2811

OTHER INFORMATION

Hazard Symbols: XI N, Risk Phrases: 43-50/53, Safety Phrases: 24-37-60-61

GENERAL DESCRIPTION OF ACCELERATOR

Sulfur combines with nearly all elements. Sulfur forms ring and chain structures as it is the second only to carbon in exhibiting catenation. The 8-membered ring and shorter chain structure of sulfur molecule is important in vulcanization process which individual polymers are linked to other polymer molecules by atomic bridges. This process produces thermoset materials which are cross-linked and irreversible substances. The term thermoplastic is for high molecular weight polymers which can undergo melting-freezing cycle. Thermosets are not melted and re-molded on heating after cured. The split of sulfur 8-membered ring structure into shorter chains provides rubber vulcanization process. The split are liked with cure sites (some of the solid bonds in the molecule) on rubber molecules, resulting in forming sulfur bridges typically between 2 and 10 atoms long. Vulcanization makes rubber harder, more durable and more resistant to heating, aging and chemical attacks. The number of sulfur atoms in the sulfur bridges varies physical properties of the end products. Short bridges containing one or two sulfur atoms offer heat resistance and long bridges offer flexible property. Vulcanization can also be accomplished with certain peroxides, gamma radiation, and several other organic compounds. The principal classes of peroxide cross-linking agents are dialkyl and diaralkyl peroxides, peroxyketals and peroxyesters. Other vulcanizing agents include amine compounds for the cross-linking of fluorocarbon rubbers, metal oxides for chlorine-containing rubbers (notably zinc oxide for chloroprene rubber) and phenol-formaldehyde resins for the production of heat-resistant butyl rubber vulcanizates. Accelerator, in the rubber industry, is added with a curing agent to speed the vulcanization. Accelerators contain sulfur and nitrogen like derivatives of benzothiazole and thiocarbanilides. The popular accelerators are sulfenamides (as a delayed-action accelerators), thiazoles, thiuram sulfides, dithocarbamates and guanidines.

There are some types of rubber accelerators. They are used in combination with each other in accordance with vulcanizing and/or acid-base conditions. Some examples classified by chemical structure are as below;

- Thiazole
  - 2-Mercaptobenzothiazole (CAS #: 149-30-4)
  - Dibenzothiazole disulfide (CAS #: 120-78-5)
  - 2-Mercaptobenzothiazole Zinc salt (CAS #: 155-04-4)
- Sulphenamide
  - N-Cyclohexyl-2-benzothiazole sulfenamide (CAS #: 95-33-0)
  - N-Oxydienthylene-2-benzothiazole sulfenamide (CAS #: 102-77-2)
  - N-tert-butyl-2-benzothiazyl sulfenamide (CAS #: 95-31-8)
- Guanidine

    - Diphenyl guanidine (CAS #: 102-06-7)
    - Di-o-tolylguanidine (CAS #: 97-39-2)
- Thiuram
    - Tetramethyl thiuram disulfide (CAS #: 137-26-8)
    - Tetraethyl thiuram disulfide (CAS #: 97-77-8)
    - Tetramethyl thiuram monosulfide (CAS #: 97-74-5)
    - Isobutyl thiuram disulfide (CAS #: 3064-73-1)
    - Tetrabenzylthiuram disulfide (CAS #: 10591-85-2)
    - Dipentamethylene thiuramtetrasulfide (CAS #: 120-54-7)
- Dithiocarbamate
    - Zinc dimethyl dithiocarbamate (CAS #: 137-30-4)
    - Zinc diethyl dithiocarbamate (CAS #: 14324-55-1)
    - Zinc dibutyl dithiocarbamate (CAS #: 136-23-2)
    - Zinc N-ethyl-dithiocarbamate (CAS #: 14634-93-6)
    - Zinc dibenzyl dithiocarbamate (CAS #: 14726-36-4)
    - Copper dimethyl dithiocarbamate (CAS #: 137-29-1)
- Thiourea
    - Ethylene thiourea (CAS #: 96-45-7)
    - N,N'-Diethylthiourea (CAS #: 105-55-5)
    - N-N'-Diphenylthiourea (CAS #: 102-08-9)