

2H-benzimidazole-2-thione, 1,3-dihydro-4(or 5)-methyl-, zinc salt

CAS# 61617-00-3

Molecular Formula: $C_{16}H_{16}N_4S_2Zn$
Molecular Weight: 393.85

1.1 GENERAL SUBSTANCE INFORMATION

- A. Type of Substance: Organic
- B. Physical State: Off-white to tan solid
- C. Purity: 95-97%

1.2 SYNONYMS Zinc mercaptotoluimidazole
Vanox® ZMTI
Vulkanox® ZMB2/C5

2. PHYSICAL-CHEMICAL DATA

2.1 MELTING POINT

Value: 300° C minimum
Decomposition: No
Sublimation: No
Method: Determination of melting point using Fisher-Johns melting point apparatus
GLP: No
Remarks: None
Reference: R. T. Vanderbilt Standard Method of Analysis (T-3B)
Reliability: (1) Valid without restriction

2.2 BOILING POINT

Value: 605° C
Pressure: 760 mm Hg
Decomposition: No data
Method: Adapted Stein and Brown method
GLP: No
Remarks: Estimation method based on molecular structure and measured melting point value.
Reference: EPIWIN/MPBPWIN v1.40
Reliability: (2) Valid with restrictions – Modelling data

2.3 DENSITY (relative density)

Type: Density
Value: 1.69
Temperature: 25° C
Method: Determination of density of solids by pycnometry
GLP: No
Remarks: None
Reference: R. T. Vanderbilt Standard Method of Analysis (T-288)

Reliability: (2) Valid with restrictions – methods other than pycnometry may be more reliable for determination of density of solids

2.4 VAPOUR PRESSURE

Value: 4.64 x 10⁻¹⁴ mm Hg
Temperature: 25 °C
Method: calculated, modified Grain method
GLP: No
Remarks: Estimation method based on molecular structure and measured melting point value.
Reference: EPIWIN/MPBPWIN v1.40
Reliability: (2) Valid with restrictions – Modelling data

2.5 PARTITION COEFFICIENT log₁₀P_{ow}

Log Pow: 3.06
Temperature: None
Method: Other: SRC LogKow (KowWin) Program
GLP: No
Remarks: Estimation method based on molecular structure fragments
Reference: EPIWIN/WSKO v1.40
Reliability: (2) Valid with restrictions – Modelling data

2.6 WATER SOLUBILITY

A Solubility

Value: 32 mg/l
Temperature: 20 °C
Description:
Method: OECD 105, OPPTS 830.7840
GLP: Yes
Test substance: As prescribed by 1.1-1.2, purity approximately 95%
Reference: R. T. Vanderbilt study 860/072
Reliability: (1) Valid without restrictions

B. pH Value, pKa Value

pH Value: Not Applicable
pKa value: Not Applicable

2.11 OXIDISING PROPERTIES

No data available.

2.12 OXIDATION: REDUCTION POTENTIAL

No data available.

2.13 ADDITIONAL DATA

A Partition co-efficient between soil/sediment and water (Kd)

B. Other data – Henry's Law Constant

Results: 7.48×10^{-16} atm-m³/mole
Remarks: Calculated at 25° C
Reference: EPIWIN/HENRYWIN v3.10
Reliability: (2) Valid with restrictions – Modelling data

3. ENVIRONMENTAL FATE AND PATHWAYS

3.1.1 PHOTODEGRADATION

Type: Air
Light source: Sunlight
Temperature: 25°C
Direct photolysis:
 Half life: 1.205 hours
 Rate constant (radical): 106.4831×10^{12} cm³/molecule-sec
Method: calculated
 Atmospheric Oxidation Program/SAR Methods, 1995
GLP: No
Test substance: As prescribed by 1.1-1.2, purity approximately 95%
Remarks: Rapid atmospheric degradation of test substance in vapor phase by reaction with photochemically produced hydroxyl radicals. Particulate test substance may be physically removed from air by both wet and dry deposition. If released to air, test substance is expected to exist primarily in particulate phase.
Reference: EPIWIN/AOPWIN v1.90

3.1.2 STABILITY IN WATER

No data available. HYDROWIN v. 1.67 could not calculate rate constants for this structure.

3.2 MONITORING DATA (ENVIRONMENTAL)

No data available

3.3 TRANSPORT AND DISTRIBUTION BETWEEN ENVIRONMENTAL COMPARTMENTS INCLUDING ESTIMATED ENVIRONMENTAL CONCENTRATIONS AND DISTRIBUTION PATHWAYS

3.3.1 TRANSPORT

Type: Adsorption
Media: Soil/Sediment
Method: Estimation method
Results: $K_{oc} = 3.22 \times 10^3$; $\log K_{oc} = 3.5081$
Remarks: None
Reference: EPIWIN/PCKOCWIN v1.66

Reliability: (2) Valid with restrictions – Modelling data

Type: Volatilization

Media: Water

Method: Estimation Method

Results: Volatilization half-life from model river: 1.55×10^{12} hours
Volatilization half-life from model lake: 1.691×10^{13} hours

Remarks: Model river = 1 m deep flowing at 1 m/sec and wind velocity of 5 m/sec. Model lake = 1 m deep flowing at 0.05 m/sec and wind velocity of 0.5 m/se.

Reference: EPIWIN/HYDROWIN v1.67

Reliability: (2) Valid with restrictions – Modelling data

3.3.2 THEORETICAL DISTRIBUTION (FUGACITY CALCULATION)

Media: Air-water-soil-sediment

Method: Fugacity level III
EPIWIN v3.10

Results:	Mass Amount (%)	Half-life (hrs)	Emissions (kg/hr)
Air	0.0172	2.41	1000
Water	18.5	1440	1000
Soil	81	1440	1000
Sediment	0.436	5760	0

Remarks: Persistence time estimated to be 1400 hours

Reference: EPISUITE/EPIWIN v3.10

Reliability: (2) Valid with restrictions – Modelling data

3.5 BIODEGRADATION

Type: aerobic

Inoculum: non-adapted sludge

Concentration of the chemical: equivalent to 5 mg/l carbon

Medium: defined culture medium

Degradation: 27% CO₂ production after 28 days

Results: not readily biodegradable but ultimately biodegradable

Method: OECD 301B, EPA 835.3110

GLP: Yes

Test substance: As prescribed by 1.1-1.2, purity approximately 95%

Remarks: Test material was toxic to non-adapted organisms at recommended concentration of 10 mg/l carbon.

Reference: R. T. Vanderbilt study 860-081

Reliability: (1) valid without restrictions.

3.6 BOD5, COD OR RATIO BOD5/COD

No data available.

3.7 BIOACCUMULATION

Species: None (estimation)

BCF: 45.7

Type of test: Calculated

GLP: No data

Test substance: As prescribed by 1.1-1.2, purity approximately 95%

Remarks: None

Reference: BCFWIN v2.14

Reliability: (2) valid with restrictions – modelling data
4. **ECOTOXICITY**

4.1 **ACUTE/PROLONGED TOXICITY TO FISH**

No data available.

4.2 **ACUTE TOXICITY TO AQUATIC INVERTEBRATES**

No data available.

4.3 **TOXICITY TO AQUATIC PLANTS, e.g. algae**

No data available.

5. **TOXICITY**

5.1 **ACUTE TOXICITY**

5.1.1 **ACUTE ORAL TOXICITY**

Type: LD₅₀
Species/strain: Rat, Sherman-Wistar
Value: 800 mg/kg b.w.
Sex: Male
of Animals: Five per group
Vehicle: Corn Oil
Doses: 0, 0.5, 1.0, 2.0, 4.0, 8.0 ml/kg b.w.
Method: Other
GLP: No
Test substance: As prescribed by 1.1-1.2, purity approximately 95%
Remarks: Test material was administered as a 25% w/v suspension in corn oil. Graded doses were administered to five groups of five male adult rats. At 4.0 ml/kg (1.0 g/kg) animals were severely depressed within 12 hours of dosing; at 8.0 ml/kg, all animals died within the first day. No abnormalities were observed in any test animal on necropsy.
Reference: R. T. Vanderbilt study 06/07/1977
Reliability: (1) Valid without restriction.

5.1.2 **ACUTE INHALATION TOXICITY**

Type: LC₅₀ (4 hr)
Species/strain: Rat, Sprague-Dawley
Value: > 2.03 mg/l
Sex: Male and female
of Animals: Five per group
Doses: 0, 2.13 mg/l
Method: OECD 073, OPPTS 870.1300
GLP: Yes
Test substance: As prescribed by 1.1-1.2, purity approximately 95%

Remarks: Test material was administered by nose-only exposure. Mass median aerodynamic diameter was 3.08 μ . There were no fatalities.
Reference: R. T. Vanderbilt study 860-073
Reliability: (1) Valid without restriction.

5.1.3 ACUTE DERMAL TOXICITY

Type: LD₅₀
Species/strain: Rat, Sprague-Dawley
Sex: Male/female
of Animals: Five per sex
Vehicle: None; arachis oil used to moisten the test material
Doses: 2,000 mg/kg b.w.
Exposure Time: 24 Hours
Value: >2,000 mg/kg bow.
Method: OECD 402, limit dose
GLP: Yes
Test substance: As prescribed by 1.1-1.2, purity approximately 95%.
Remarks: Test material was moistened with arachis oil and applied to an area of shorn skin. All test animals received a single dermal exposure of 2,000 mg/kg b.w. The test material was held in place by surgical gauze and self-adhesive bandage. The semi-occlusive wrap was removed after 24 hours and the excess material was wiped from the test animal. There were no deaths, no signs of systemic toxicity, no signs of dermal irritation and all animals showed expected weight gain. No abnormalities were noted at necropsy
Reference: R. T. Vanderbilt study 860-074
Reliability: (1) Valid without restriction

5.2 CORROSIVENESS/IRRITATION

5.2.1 SKIN IRRITATION/CORROSION

Species/Strain: Rabbits, New Zealand Albino
Results: Slightly irritating
Classification: Not irritating
Method: Draize, J.H., Woodard, G., and Calvery, H.O., 1944
GLP: Yes
Test substance: As prescribed by 1.1-1.2, purity approximately 95%
Remarks: The skin on the dorsal surface of six animals was shaved with an electric clipper. The skin on one side of the animal was abraded with a lancet, sufficiently deep to penetrate the stratum corneum but not deep enough to cause bleeding. One-half (0.5) gram of test material was applied to each of two intact and two abraded sites on each animal. Test material was applied to the skin under gauze patches and held in contact with the skin by an occlusive wrap. The occlusive wrap and gauze patches were removed after 24 hours. Treated areas were examined when test material was removed and 48 hours thereafter. Irritation was scored by the Draize Method; all scores were zero.
Reference: R. T. Vanderbilt study 06/07/1977

Reliability:

(2) Valid with restrictions – Differs from current testing guidelines by using abraded skin surface, a 24-hr contact period rather than a 4-hr contact period.

5.2.2 EYE IRRITATION/CORROSION

Species/strain: Rabbits, New Zealand Albino
Results: Slightly irritating
Classification: Not irritating
Method: Draize, J.H., Woodard, G., and Calvery, H.O., 1944
GLP: Yes
Test substance: As prescribed in 1.1-1.2, purity approximately 95%
Remarks: One-tenth (0.1) gram test material was instilled into the conjunctival sac of the right eye of each animal; the left eye remained untreated as control. Test material was not washed from the eyes. Observations for signs of irritation were conducted one hour after application and 1, 2, 3, 5 and 7 days after dosing. The Draize Method was used for scoring eye irritation. The average Draize score for 24, 48 and 72 hours was calculated for each animal and then averaged over the six animals. The average Draize score was 0.3 on a scale from 0-110. All signs of irritation had subsided by the second day after exposure.
Reference: R. T. Vanderbilt study 06/07/1977
Reliability: (1) Valid without restriction

5.4 REPEATED DOSE TOXICITY

No data available.

5.5 GENETIC TOXICITY IN VITRO

A BACTERIAL TEST

Type: Ames Bacterial Reverse Mutation Assay
System of testing: Salmonella typhimurium TA1535, TA1537, TA102, TA98, TA100
Concentration: 0, 50, 150, 500, 1500 and 5000 µg/plate
Metabolic activation: With and Without
Results:
Cytotoxic conc.: With metabolic activation: 5,000 µg/plate
Without metabolic activation: 5,000 µg/plate
Precipitate conc.: >5,000 µg/plate
Genotoxic effects:
With metabolic activation: negative
Without metabolic activation: negative
Method: Ames *et al.*, Mutation Res. 31: 347-364 (1975); OECD 471
GLP: Yes
Test substance: As prescribed in 1.1-1.2, purity approximately 95%
Remarks: The test compound was evaluated for genetic activity in microbial assays with and without the addition of mammalian metabolic activation preparations. The *Salmonella typhimurium* strains used for this experiment were obtained from the University of California at Berkeley. The activation system used was S-9 homogenate from adult male Sprague-Dawley rat livers induced with phenobarbitone and β-naphthoflavone. Positive controls for the non-activation assays were N-ethyl-N'-nitro-N-nitrosoguanidine, 9-aminoacridine, mitomycin C and 4-

nitroquinoline-1-oxide. Positive control chemicals used for the activation assays were 2-aminoanthracene, benzo(a)pyrene, and 1.8-dihydroxyanthraquinone.

Non-activation results: No mutagenic activity in any indicator organism at any dose.

Activation results: No mutagenic activity in any indicator organism at any dose.

A slight decrease in the frequency of revertant colonies was observed at the high dose.

Reference: R. T. Vanderbilt study 860-077
Reliability: (1) Valid without restriction

B. NON-BACTERIAL IN VITRO TEST

No data available.

5.6 GENETIC TOXICITY IN VIVO

No data available.

5.7 CARCINOGENICITY

No data available.

5.8 TOXICITY TO REPRODUCTION

No data available.

5.9 DEVELOPMENTAL TOXICITY/ TERATOGENICITY

No data available.

5.10 OTHER RELEVANT INFORMATION

A. Specific toxicities

No data available.

B. Toxicodynamics, toxicokinetics

No data available.

5.11 EXPERIENCE WITH HUMAN EXPOSURE

No data available.