

1 Identification

Product identifier

Product name: Bis(pentamethylcyclopentadienyl)zirconiumdichloride

Stock number: 39555

CAS Number:

54039-38-2

Relevant identified uses of the substance or mixture and uses advised against.

Identified use: SU24 Scientific research and development

Details of the supplier of the safety data sheet

Manufacturer/Supplier:

Alfa Aesar
 Thermo Fisher Scientific Chemicals, Inc.
 30 Bond Street
 Ward Hill, MA 01835-8099
 Tel: 800-343-0660
 Fax: 800-322-4757
 Email: tech@alfa.com
 www.alfa.com

Information Department: Health, Safety and Environmental Department

Emergency telephone number:

During normal business hours (Monday-Friday, 8am-7pm EST), call (800) 343-0660. After normal business hours, call Carechem 24 at (866) 928-0789.

2 Hazard(s) identification

Classification of the substance or mixture in accordance with 29 CFR 1910 (OSHA HCS)



GHS02 Flame

Water-react. 2 H261 In contact with water releases flammable gas.



GHS06 Skull and crossbones

Acute Tox. 3 H301 Toxic if swallowed.

Acute Tox. 3 H311 Toxic in contact with skin.



GHS05 Corrosion

Skin Corr. 1B H314 Causes severe skin burns and eye damage.

Eye Dam. 1 H318 Causes serious eye damage.



GHS07

Acute Tox. 4 H332 Harmful if inhaled.

Hazards not otherwise classified No information known.

Label elements

GHS label elements The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)

Hazard pictograms



GHS02 GHS05 GHS06

Signal word

Danger

Hazard statements

H261 In contact with water releases flammable gas.

H301+H311 Toxic if swallowed or in contact with skin.

H332 Harmful if inhaled.

H314 Causes severe skin burns and eye damage.

Precautionary statements

P231+P232 Handle under inert gas. Protect from moisture.

P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/ doctor/...

P303+P361+P353 If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P361 Take off immediately all contaminated clothing.

P405 Store locked up.

P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

WHMIS classification

B6 - Reactive flammable material

D2B - Toxic material causing other toxic effects

E - Corrosive material



Classification system

HMIS ratings (scale 0-4)

(Hazardous Materials Identification System)

HEALTH 3 Health (acute effects) = 3

FIRE 1 Flammability = 1

REACTIVITY 2 Physical Hazard = 2

Other hazards

Results of PBT and vPvB assessment

PBT: Not applicable.

Product name: **Bis(pentamethylcyclopentadienyl)zirconiumdichloride**

vPvB: Not applicable.

(Contd. of page 1)

3 Composition/information on ingredients

Chemical characterization: Substances

CAS# Description:

54039-38-2 Bis(pentamethylcyclopentadienyl)zirconiumdichloride

Additional information: Zirconium is routinely found with a low level of hafnium since separation of the two elements is difficult.

4 First-aid measures

Description of first aid measures

General information Immediately remove any clothing soiled by the product.

After inhalation

Supply fresh air. If required, provide artificial respiration. Keep patient warm.

Seek immediate medical advice.

After skin contact

Immediately wash with water and soap and rinse thoroughly.

Seek immediate medical advice.

After eye contact Rinse opened eye for several minutes under running water. Then consult a doctor.

After swallowing Seek medical treatment.

Information for doctor

Most important symptoms and effects, both acute and delayed

Causes severe skin burns.

Causes serious eye damage.

Indication of any immediate medical attention and special treatment needed No further relevant information available.

5 Fire-fighting measures

Extinguishing media

Suitable extinguishing agents CO₂, sand, extinguishing powder. Do not use water.

For safety reasons unsuitable extinguishing agents Water

Special hazards arising from the substance or mixture

Reacts violently with water

If this product is involved in a fire, the following can be released:

Carbon monoxide and carbon dioxide

Metal oxide fume

Hydrogen chloride (HCl)

Advice for firefighters

Protective equipment:

Wear self-contained respirator.

Wear fully protective impervious suit.

6 Accidental release measures

Personal precautions, protective equipment and emergency procedures

Wear protective equipment. Keep unprotected persons away.

Ensure adequate ventilation

Environmental precautions: Do not allow material to be released to the environment without proper governmental permits.

Methods and material for containment and cleaning up:

Use neutralizing agent.

Dispose of contaminated material as waste according to section 13.

Ensure adequate ventilation.

Do not flush with water or aqueous cleansing agents

Prevention of secondary hazards: No special measures required.

Reference to other sections

See Section 7 for information on safe handling

See Section 8 for information on personal protection equipment.

See Section 13 for disposal information.

7 Handling and storage

Handling

Precautions for safe handling

Handle under dry protective gas.

Keep container tightly sealed.

Store in cool, dry place in tightly closed containers.

Ensure good ventilation at the workplace.

Information about protection against explosions and fires: No information known.

Conditions for safe storage, including any incompatibilities

Storage

Requirements to be met by storerooms and receptacles: No special requirements.

Information about storage in one common storage facility:

Store away from oxidizing agents.

Store away from strong bases.

Store away from air.

Store away from water/moisture.

Further information about storage conditions:

Store under dry inert gas.

This product is moisture sensitive.

This product is air sensitive.

Protect from humidity and water.

Keep container tightly sealed.

Store in cool, dry conditions in well sealed containers.

Specific end use(s) No further relevant information available.

8 Exposure controls/personal protection

Additional information about design of technical systems:

Properly operating chemical fume hood designed for hazardous chemicals and having an average face velocity of at least 100 feet per minute.

Control parameters

Components with limit values that require monitoring at the workplace:

Zirconium and compounds, as Zr
mg/m³

(Contd. on page 3)
USA

Product name: Bis(pentamethylcyclopentadienyl)zirconiumdichloride

(Contd. of page 2)

ACGIH TLV 5; 10-STEL
Austria MAK 5
Denmark TWA 5
Finland TWA 5
Hungary 5-STEL
Korea TLV 5
Poland TWA 5; 10-STEL
Russia 5-STEL
OSHA PEL 5

Additional information: No data

Exposure controls

Personal protective equipment

General protective and hygienic measures

The usual precautionary measures for handling chemicals should be followed.

Keep away from foodstuffs, beverages and feed.

Remove all soiled and contaminated clothing immediately.

Wash hands before breaks and at the end of work.

Avoid contact with the eyes and skin.

Maintain an ergonomically appropriate working environment.

Breathing equipment: Use suitable respirator when high concentrations are present.

Protection of hands:

Impervious gloves

Check protective gloves prior to each use for their proper condition.

The selection of suitable gloves not only depends on the material, but also on quality. Quality will vary from manufacturer to manufacturer.

Penetration time of glove material (in minutes) Not determined

Eye protection:

Tightly sealed goggles

Full face protection

Body protection: Protective work clothing.

9 Physical and chemical properties

Information on basic physical and chemical properties

General Information

Appearance:

Form: Crystalline
Color: Pale yellow
Odor: Not determined
Odor threshold: Not determined.

pH-value: Not applicable.

Change in condition

Melting point/Melting range: Not determined
Boiling point/Boiling range: Not determined
Sublimation temperature / start: Not determined
Flammability (solid, gaseous) Not determined.
Ignition temperature: Not determined
Decomposition temperature: Not determined
Auto igniting: Not determined.

Danger of explosion: Product does not present an explosion hazard.

Explosion limits:

Lower: Not determined
Upper: Not determined
Vapor pressure: Not applicable.
Density: Not determined
Relative density Not determined.
Vapor density Not applicable.
Evaporation rate Not applicable.

Solubility in / Miscibility with

Water: Reacts violently
Partition coefficient (n-octanol/water): Not determined.
Viscosity:
dynamic: Not applicable.
kinematic: Not applicable.
Other information No further relevant information available.

10 Stability and reactivity

Reactivity Reacts violently with water.

Chemical stability Stable under recommended storage conditions.

Thermal decomposition / conditions to be avoided: Decomposition will not occur if used and stored according to specifications.

Possibility of hazardous reactions Reacts violently with water

Conditions to avoid No further relevant information available.

Incompatible materials:

Oxidizing agents

Bases

Air

Water/moisture

Hazardous decomposition products:

Carbon monoxide and carbon dioxide

Metal oxide fume

Hydrogen chloride (HCl)

11 Toxicological information

Information on toxicological effects

Acute toxicity:

Harmful if inhaled.

Toxic in contact with skin.

Toxic if swallowed.

Danger through skin absorption.

Swallowing will lead to a strong corrosive effect on mouth and throat and to the danger of perforation of esophagus and stomach.

LD/LC50 values that are relevant for classification: No data

(Contd. on page 4)
USA

Product name: **Bis(pentamethylcyclopentadienyl)zirconiumdichloride**

(Contd. of page 3)

Skin irritation or corrosion: Causes severe skin burns.
Eye irritation or corrosion: Causes serious eye damage.
Sensitization: No sensitizing effects known.
Germ cell mutagenicity: No effects known.
Carcinogenicity: No classification data on carcinogenic properties of this material is available from the EPA, IARC, NTP, OSHA or ACGIH.
Reproductive toxicity: No effects known.
Specific target organ system toxicity - repeated exposure: No effects known.
Specific target organ system toxicity - single exposure: No effects known.
Aspiration hazard: No effects known.
Subacute to chronic toxicity: Inhalation of zirconium compounds may cause pulmonary granulomas.
Subacute to chronic toxicity: No effects known.
Additional toxicological information: To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.

12 Ecological information

Toxicity
Aquatic toxicity: No further relevant information available.
Persistence and degradability No further relevant information available.
Bioaccumulative potential No further relevant information available.
Mobility in soil No further relevant information available.
Additional ecological information:
General notes:
Do not allow material to be released to the environment without proper governmental permits.
Do not allow undiluted product or large quantities to reach ground water, water course or sewage system.
Avoid transfer into the environment.
Results of PBT and vPvB assessment
PBT: Not applicable.
vPvB: Not applicable.
Other adverse effects No further relevant information available.

13 Disposal considerations

Waste treatment methods
Recommendation Consult state, local or national regulations to ensure proper disposal.
Uncleaned packagings:
Recommendation: Disposal must be made according to official regulations.

14 Transport information

UN-Number DOT, IMDG, IATA	UN3096
UN proper shipping name DOT	Corrosive solids, water-reactive, n.o.s. (Bis(pentamethylcyclopentadienyl)zirconiumdichloride)
IMDG, IATA	CORROSIVE SOLID, WATER-REACTIVE, N.O.S. (Bis(pentamethylcyclopentadienyl)zirconiumdichloride)
Transport hazard class(es) DOT	
Class Label Class Label IMDG, IATA	8 Corrosive substances. 8+4.3 8 (CW2) Corrosive substances 8+4.3
Class Label	8 Corrosive substances. 8+4.3
Packing group DOT, IMDG, IATA	II
Environmental hazards:	Not applicable.
Special precautions for user EMS Number:	Warning: Corrosive substances F-G,S-L
Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code	Not applicable.
Transport/Additional information: DOT Marine Pollutant (DOT):	No
UN "Model Regulation":	UN3096, Corrosive solids, water-reactive, n.o.s. (Bis(pentamethylcyclopentadienyl)zirconiumdichloride), 8 (4.3), II

15 Regulatory information

Safety, health and environmental regulations/legislation specific for the substance or mixture
GHS label elements The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)
Hazard pictograms



GHS02 GHS05 GHS06

Signal word Danger
Hazard statements

H261 In contact with water releases flammable gas.

(Contd. on page 5)
USA

Product name: Bis(pentamethylcyclopentadienyl)zirconiumdichloride

(Contd. of page 4)

H301+H311 Toxic if swallowed or in contact with skin.
H332 Harmful if inhaled.
H314 Causes severe skin burns and eye damage.

Precautionary statements

P231+P232 Handle under inert gas. Protect from moisture.
P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/ doctor/...
P303+P361+P353 If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P361 Take off immediately all contaminated clothing.
P405 Store locked up.
P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

National regulations

This product is not listed in the U.S. Environmental Protection Agency Toxic Substances Control Act Chemical Substance Inventory. Use of this product is restricted to research and development only. This product must be used by or directly under the supervision of a technically qualified individual as defined by TSCA. This product must not be used for commercial purposes or in formulations for commercial purposes.

SARA Section 313 (specific toxic chemical listings) Substance is not listed.

California Proposition 65

Prop 65 - Chemicals known to cause cancer Substance is not listed.

Prop 65 - Developmental toxicity Substance is not listed.

Prop 65 - Developmental toxicity, female Substance is not listed.

Prop 65 - Developmental toxicity, male Substance is not listed.

Information about limitation of use: For use only by technically qualified individuals.

Other regulations, limitations and prohibitive regulations

Substance of Very High Concern (SVHC) according to the REACH Regulations (EC) No. 1907/2006. Substance is not listed.

The conditions of restrictions according to Article 67 and Annex XVII of the Regulation (EC) No 1907/2006 (REACH) for the manufacturing, placing on the market and use must be observed.

Substance is not listed.

Annex XIV of the REACH Regulations (requiring Authorisation for use) Substance is not listed.

Chemical safety assessment: A Chemical Safety Assessment has not been carried out.

16 Other information

Employers should use this information only as a supplement to other information gathered by them, and should make independent judgement of suitability of this information to ensure proper use and protect the health and safety of employees. This information is furnished without warranty, and any use of the product not in conformance with this Material Safety Data Sheet, or in combination with any other product or process, is the responsibility of the user.

Department issuing SDS: Global Marketing Department

Date of preparation / last revision 11/24/2015 / -

Abbreviations and acronyms:

RID: Règlement international concernant le transport des marchandises dangereuses par chemin de fer (Regulations Concerning the International Transport of Dangerous Goods by Rail)

IATA-DGR: Dangerous Goods Regulations by the "International Air Transport Association" (IATA)

ICAO: International Civil Aviation Organization

ICAO-TI: Technical Instructions by the "International Civil Aviation Organization" (ICAO)

ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)

IMDG: International Maritime Code for Dangerous Goods

DOT: US Department of Transportation

IATA: International Air Transport Association

CAS: Chemical Abstracts Service (division of the American Chemical Society)

HMIS: Hazardous Materials Identification System (USA)

WHMIS: Workplace Hazardous Materials Information System (Canada)

LC50: Lethal concentration, 50 percent

LD50: Lethal dose, 50 percent

vPvB: very Persistent and very Bioaccumulative

ACGIH: American Conference of Governmental Industrial Hygienists (USA)

OSHA: Occupational Safety and Health Administration (USA)

NTP: National Toxicology Program (USA)

IARC: International Agency for Research on Cancer

EPA: Environmental Protection Agency (USA)