

ALFAA39405

t-Butylferrocene

SECTION 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

| | |
|---|--|
| 产品说明: Product Description: | 叔丁基二茂铁 t-Butylferrocene |
| Cat No. : | 39405 |
| CAS No | 1316-98-9 |
| Molecular Formula | C14 H18 Fe |
| Supplier | Avocado Research Chemicals Ltd. (Part of Thermo Fisher Scientific) Shore Road, Heysham Lancashire, LA3 2XY, United Kingdom Office Tel: +44 (0) 1524 850506 Office Fax: +44 (0) 1524 850608 |
| Emergency Telephone Number | For information US call: 001-800-227-6701 / Europe call: +32 14 57 52 11 Emergency Number US :001-201-796-7100 / Europe : +32 14 57 52 99 CHEMTREC Tel. No. US :001-800-424-9300 / Europe :001-703-527-3887 |
| E-mail address | begel.sdsdesk@thermofisher.com |
| Recommended Use Uses advised against | Laboratory chemicals. No Information available |

SECTION 2. HAZARD IDENTIFICATION

Physical State
Liquid

Appearance
Dark orange

Odor
No information available

Emergency Overview

The product contains no substances which at their given concentration are considered to be hazardous to health.

Classification of the substance or mixture

Based on available data, the classification criteria are not met

Label Elements

None required

Physical and Chemical Hazards

None identified.

Health Hazards

The product contains no substances which at their given concentration are considered to be hazardous to health.

Environmental hazards

Contains no substances known to be hazardous to the environment or not degradable in waste water treatment plants. Will likely be mobile in the environment due to its volatility. The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces.

This product does not contain any known or suspected endocrine disruptors.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

| Component | CAS No | Weight % |
|------------------|-----------|----------|
| t-Butylferrocene | 1316-98-9 | <=100 |

SECTION 4. FIRST AID MEASURES**Eye Contact**

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

Skin Contact

Wash off immediately with plenty of water for at least 15 minutes. Get medical attention immediately if symptoms occur.

Inhalation

Remove to fresh air. Get medical attention immediately if symptoms occur.

Ingestion

Clean mouth with water and drink afterwards plenty of water. Get medical attention if symptoms occur.

Most important symptoms and effects

None reasonably foreseeable.

Self-Protection of the First Aider

No special precautions required.

Notes to Physician

Treat symptomatically.

SECTION 5. FIRE-FIGHTING MEASURES**Suitable Extinguishing Media**

Use extinguishing measures that are appropriate to local circumstances and the surrounding environment.

Extinguishing media which must not be used for safety reasons

No information available.

Specific Hazards Arising from the Chemical

Thermal decomposition can lead to release of irritating gases and vapors.

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

SECTION 6. ACCIDENTAL RELEASE MEASURES**Personal Precautions**

Ensure adequate ventilation. Use personal protective equipment as required.

Environmental Precautions

Should not be released into the environment. See Section 12 for additional Ecological Information.

Methods for Containment and Clean Up

t-Butylferrocene

Sweep up and shovel into suitable containers for disposal.

Refer to protective measures listed in Sections 8 and 13.

SECTION 7. HANDLING AND STORAGE

Handling

Wear personal protective equipment/face protection. Ensure adequate ventilation. Avoid contact with skin, eyes or clothing. Avoid ingestion and inhalation.

Storage

Keep container tightly closed in a dry and well-ventilated place.

Specific Use(s)

Use in laboratories

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Control Parameters

Monitoring methods

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents. MDHS70 General methods for sampling airborne gases and vapours MDHS 88 Volatile organic compounds in air. Laboratory method using diffusive samplers, solvent desorption and gas chromatography MDHS 96 Volatile organic compounds in air - Laboratory method using pumped solid sorbent tubes, solvent desorption and gas chromatography

Exposure Controls

Engineering Measures

None under normal use conditions.

Personal protective equipment

| | |
|------------------------|---|
| Eye Protection | Wear safety glasses with side shields (or goggles) (European standard - EN 166) |
| Hand Protection | Protective gloves |

| Glove material | Breakthrough time | Glove thickness | EU standard | Glove comments |
|----------------|-----------------------------------|-----------------|-------------|-----------------------|
| Nitrile rubber | See manufacturers recommendations | - | EN 374 | (minimum requirement) |
| Neoprene | | | | |
| Natural rubber | | | | |
| PVC | | | | |

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

| | |
|----------------------------------|--|
| Skin and body protection | Long sleeved clothing |
| Respiratory Protection | No protective equipment is needed under normal use conditions. |
| Large scale/emergency use | Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced Recommended Filter type: Particle filter |

t-Butylferrocene

Small scale/Laboratory use Maintain adequate ventilation
Recommended half mask:- Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141

Hygiene Measures Handle in accordance with good industrial hygiene and safety practice.

Environmental exposure controls No information available.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

| | | |
|--|------------------------------------|--|
| Appearance | Dark orange | |
| Physical State | Liquid | |
| Odor | No information available | |
| Odor Threshold | No data available | |
| pH | No information available | |
| Melting Point/Range | No data available | |
| Softening Point | No data available | |
| Boiling Point/Range | 80 °C / 176 °F | |
| Flash Point | > 109 °C / > 228.2 °F | Method - No information available |
| Evaporation Rate | No data available | |
| Flammability (solid,gas) | Not applicable | Liquid |
| Explosion Limits | No data available | |
| Vapor Pressure | No data available | |
| Vapor Density | No data available | (Air = 1.0) |
| Specific Gravity / Density | 1.201 g/cm ³ | @ 20 °C |
| Bulk Density | Not applicable | Liquid |
| Water Solubility | Immiscible | |
| Solubility in other solvents | No information available | |
| Partition Coefficient (n-octanol/water) | | |
| Autoignition Temperature | No data available | |
| Decomposition Temperature | No data available | |
| Viscosity | No data available | |
| Explosive Properties | No information available | |
| Oxidizing Properties | No information available | |
| Molecular Formula | C ₁₄ H ₁₈ Fe | |
| Molecular Weight | 242.15 | |

SECTION 10. STABILITY AND REACTIVITY

Stability Stable under normal conditions.

Hazardous Reactions None under normal processing.

Hazardous Polymerization No information available.

Conditions to Avoid None known.

Materials to avoid No information available.

Hazardous Decomposition Products None under normal use conditions.

SECTION 11. TOXICOLOGICAL INFORMATION

Product Information

SAFETY DATA SHEET

t-Butylferrocene

| | |
|---|---|
| (a) acute toxicity; | |
| (b) skin corrosion/irritation; | No data available |
| (c) serious eye damage/irritation; | No data available |
| (d) respiratory or skin sensitization; | |
| Respiratory | No data available |
| Skin | No data available |
| (e) germ cell mutagenicity; | No data available |
| (f) carcinogenicity; | No data available |
| | There are no known carcinogenic chemicals in this product |
| (g) reproductive toxicity; | No data available |
| (h) STOT-single exposure; | No data available |
| (i) STOT-repeated exposure; | No data available |
| Target Organs | No information available. |
| (j) aspiration hazard; | No data available |
| Symptoms / effects, both acute and delayed | No information available |

SECTION 12. ECOLOGICAL INFORMATION

| | |
|--|--|
| Ecotoxicity effects | Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants. |
| Persistence and Degradability | |
| Persistence | Persistence is unlikely, based on information available. |
| Bioaccumulative Potential | Bioaccumulation is unlikely |
| Mobility in soil | The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces. Will likely be mobile in the environment due to its volatility. Disperses rapidly in air. |
| Endocrine Disruptor Information | This product does not contain any known or suspected endocrine disruptors |
| Persistent Organic Pollutant | This product does not contain any known or suspected substance |
| Ozone Depletion Potential | This product does not contain any known or suspected substance |

SECTION 13. DISPOSAL CONSIDERATIONS

t-Butylferrocene

| | |
|--|---|
| Waste from Residues/Unused Products | Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification. |
| Contaminated Packaging | Empty remaining contents. Dispose of in accordance with local regulations. Do not re-use empty containers. |
| Other Information | Waste codes should be assigned by the user based on the application for which the product was used. |

SECTION 14. TRANSPORT INFORMATION

| | |
|-------------------------------------|---------------------------------|
| Road and Rail Transport | Not Regulated |
| IMDG/IMO | Not regulated |
| IATA | Not regulated |
| Special Precautions for User | No special precautions required |

SECTION 15. REGULATORY INFORMATION

International Inventories

X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), Korea (KECL).

| Component | The Inventory of Hazardous Chemicals (2015 Edition) | List of dangerous goods GB 12268 - 2012 | TCSI | IECSC | EINECS | TSCA | DSL | PICCS | ENCS | ISHL | AICS | KECL |
|------------------|---|---|------|-------|--------|------|-----|-------|------|------|------|------|
| t-Butylferrocene | - | - | X | - | - | - | - | - | - | - | - | - |

National Regulations

SECTION 16. OTHER INFORMATION

| | |
|-------------------------|---|
| Prepared By | Health, Safety and Environmental Department |
| Revision Date | 07-Oct-2025 |
| Revision Summary | Not applicable. |

Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Legend

CAS - Chemical Abstracts Service

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

DSL/NDSL - Canadian Domestic Substances List/Non-Domestic Substances List

t-Butylferrocene

PICCS - Philippines Inventory of Chemicals and Chemical Substances
IECSC - Chinese Inventory of Existing Chemical Substances
KECL - Korean Existing and Evaluated Chemical Substances

ENCS - Japanese Existing and New Chemical Substances
AICS - Australian Inventory of Chemical Substances
NZIoC - New Zealand Inventory of Chemicals

WEL - Workplace Exposure Limit
ACGIH - American Conference of Governmental Industrial Hygienists
DNEL - Derived No Effect Level
RPE - Respiratory Protective Equipment
LC50 - Lethal Concentration 50%
NOEC - No Observed Effect Concentration
PBT - Persistent, Bioaccumulative, Toxic

TWA - Time Weighted Average
IARC - International Agency for Research on Cancer
PNEC - Predicted No Effect Concentration
LD50 - Lethal Dose 50%
EC50 - Effective Concentration 50%
POW - Partition coefficient Octanol:Water
vPvB - very Persistent, very Bioaccumulative

ICAO/IATA - International Civil Aviation Organization/International Air Transport Association
ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road
OECD - Organisation for Economic Co-operation and Development
BCF - Bioconcentration factor

IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code
MARPOL - International Convention for the Prevention of Pollution from Ships
ATE - Acute Toxicity Estimate
VOC - (Volatile Organic Compound)

Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>
Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of Safety Data Sheet