

SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifier**

Trade name

Benzylzinc bromide, 0.5M in THF

Stock number:

H58014

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

Identified use:

SU24 Scientific research and development

1.3 Details of the supplier of the safety data sheet

Manufacturer/Supplier:

Alfa Aesar GmbH & Co.KG
A Johnson Matthey Company
Zeppelinstr. 7b
76185 Karlsruhe / Germany
Tel: +49 (0) 721 84007 280
Fax: +49 (0) 721 84007 300
Email: tech@alfa.com
www.alfa.com

Informing department:

Product safety Tel + +049 (0) 7275 988687-0

1.4 Emergency telephone number:

Carechem 24: +44 (0) 1235 239 670 (Multi-language emergency number)

Poison Information Center Mainz

www.giftinfo.uni-mainz.de Telephone: +49(0)6131/19240

SECTION 2: Hazards identification**2.1 Classification of the substance or mixture**

Classification according to Regulation (EC) No 1272/2008



GHS02 flame

Flam. Liq. 2 H225 Highly flammable liquid and vapour.

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



GHS08 health hazard

Carc. 2 H351 Suspected of causing cancer.



GHS05 corrosion

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



GHS07

STOT SE 3 H335 May cause respiratory irritation.

Classification according to Directive 67/548/EEC or Directive 1999/45/EC

C; Corrosive

R34: Causes burns.

F; Highly flammable

R11: Highly flammable.

R14-19: Reacts violently with water. May form explosive peroxides.

Information concerning particular hazards for human and environment:

The product has to be labelled due to the calculation procedure of the "General Classification guideline for preparations of the EU" in the latest valid version.

Other hazards that do not result in classification

No information known.

2.2 Label elements**Labelling according to Regulation (EC) No 1272/2008**

Hazard pictograms

Signal word

The product is classified and labelled according to the CLP regulation.

GHS02, GHS05, GHS07, GHS08

Danger

Hazard-determining components of labelling:

Tetrahydrofuran
Benzylzinc bromide

Hazard statements

H225 Highly flammable liquid and vapour.
H261 In contact with water releases flammable gases.
H314 Causes severe skin burns and eye damage.
H351 Suspected of causing cancer.
H335 May cause respiratory irritation.

Precautionary statements

P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
P231+P232 Handle under inert gas. Protect from moisture.
P303+P361+P353 IF ON SKIN (or hair): Remove/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.
P405 Store locked up.
P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

Additional information:

EUH014 Reacts violently with water.
EUH019 May form explosive peroxides.

2.3 Other hazards

Results of PBT and vPvB assessment

PBT:

Not applicable.

vPvB:

Not applicable.

SECTION 3: Composition/information on ingredients**3.2 Mixtures****Dangerous components:**

CAS: 109-99-9 EINECS: 203-726-8	Tetrahydrofuran	Xn R40; Xi R36/37; F R11 R19 Flam. Liq. 2, H225; Carc. 2, H351; Eye Irrit. 2, H319; STOT SE 3, H335	88,2%
CAS: 62673-31-8	Benzylzinc bromide	C R34 R14 Skin Corr. 1B, H314	11,8%

Additional information

None known.

Trade name **Benzylzinc bromide, 0.5M in THF**

(Contd. of page 1)

SECTION 4: First aid measures**4.1 Description of first aid measures****General information****After inhalation**

Instantly remove any clothing soiled by the product.
Supply fresh air. If required, provide artificial respiration. Keep patient warm. Consult doctor if symptoms persist.

Seek immediate medical advice.

Instantly wash with water and soap and rinse thoroughly.

Seek immediate medical advice.

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

Seek medical treatment.

After skin contact**After eye contact****After swallowing****4.2 Most important symptoms and effects, both acute and delayed**

No further relevant information available.

4.3 Indication of any immediate medical attention and special treatment needed

No further relevant information available.

SECTION 5: Firefighting measures**5.1 Extinguishing media****Suitable extinguishing agents**

CO₂, extinguishing powder or water jet. Fight larger fires with water jet or alcohol-resistant foam.

For safety reasons unsuitable extinguishing agents

Water.

5.2 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

Hydrogen bromide (HBr)

Metal oxide

5.3 Advice for firefighters**Protective equipment:**

Wear self-contained breathing apparatus.

Wear full protective suit.

SECTION 6: Accidental release measures**6.1 Personal precautions, protective equipment and emergency procedures**

Wear protective equipment. Keep unprotected persons away.

Ensure adequate ventilation

Keep away from ignition sources

6.2 Environmental precautions:

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

Do not allow product to reach sewage system or water bodies.

Do not allow to enter the ground/soil.

6.3 Methods and material for containment and cleaning up:

Keep away from ignition sources.

Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).

Use neutralizing agent.

Dispose of contaminated material as waste according to item 13.

Ensure adequate ventilation.

Do not flush with water or aqueous cleansing agents

Keep away from ignition sources.

Prevention of secondary hazards:**6.4 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 information on disposal.

SECTION 7: Handling and storage**7.1 Precautions for safe handling**

Handle under dry protective gas.

Keep containers tightly sealed.

Ensure good ventilation/exhaustion at the workplace.

Open and handle container with care.

Information about protection against explosions and fires:

Protect against electrostatic charges.

Fumes can combine with air to form an explosive mixture.

Do not distill to dryness.

Explosive peroxides may form, handle container cautiously.

7.2 Conditions for safe storage, including any incompatibilities**Storage****Requirements to be met by storerooms and containers:**

Refrigerate

Information about storage in one common storage facility:

Store away from water.

Store away from air.

Protect from heat.

Store away from oxidizing agents.

Further information about storage conditions:

Store under dry inert gas.

This product is air sensitive.

Protect from humidity and keep away from water.

Avoid contact with air / oxygen (formation of peroxide).

Store in a locked cabinet or with access restricted to technical experts or their assistants.

Refrigerate

Check container pressure periodically to prevent explosive peroxides.

7.3 Specific end use(s)

No further relevant information available.

SECTION 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.

8.1 Control parameters**Components with critical values that require monitoring at the workplace:****109-99-9 Tetrahydrofuran (88,2%)**

AGW (Germany) 150 mg/m³, 50 ppm
2(l);DFG, EU, H, Y

PEL (USA) 590 mg/m³, 200 ppm

(Contd. on page 3)
DE/E

Trade name Benzylzinc bromide, 0.5M in THF

(Contd. of page 2)

REL (USA)	Short-term value: 735 mg/m ³ , 250 ppm Long-term value: 590 mg/m ³ , 200 ppm
TLV (USA)	Short-term value: 295 mg/m ³ , 100 ppm Long-term value: 147 mg/m ³ , 50 ppm Skin

Ingredients with biological limit values:**109-99-9 Tetrahydrofuran (88,2%)**

BGW (Germany)	2 mg/l U b Tetrahydrofuran
BEI (USA)	2 mg/L urine end of shift Tetrahydrofuran

Additional information: No data**8.2 Exposure controls****Personal protective equipment****General protective and hygienic measures**

The usual precautionary measures should be adhered to in handling the chemicals.

Keep away from foodstuffs, beverages and food.

Instantly remove any soiled and impregnated garments.

Wash hands during breaks and at the end of the work.

Avoid contact with the eyes and skin.

Maintain an ergonomically appropriate working environment.

Use breathing protection with high concentrations.

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

The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.

Impervious gloves

Not determined

Tightly sealed safety glasses.

Full face protection

Protective work clothing.

Breathing equipment:**Protection of hands:****Material of gloves****Penetration time of glove material****Eye protection:****Body protection:****SECTION 9: Physical and chemical properties****9.1 Information on basic physical and chemical properties****General Information****Appearance:**

Form:	Liquid
Colour:	Yellow to brown to black
Smell:	Not determined
Odour threshold:	Not determined.

pH-value: Not determined.**Change in condition**

Melting point/Melting range:	Not determined
Boiling point/Boiling range:	Not determined
Sublimation temperature / start:	Not determined
Inflammability (solid, gaseous)	Not determined.
Ignition temperature:	230 °C
Decomposition temperature:	Not determined
Self-inflammability:	Product is not selfigniting.

Danger of explosion: May form explosive peroxides.
Do not distill to dryness.**Critical values for explosion:**

Lower:	1,5 Vol %
Upper:	12,0 Vol %
Steam pressure at 20 °C:	200 hPa
Density at 20 °C	0,978 g/cm ³
Relative density	Not determined.
Vapour density	Not determined.
Evaporation rate	Not determined.
Solubility in / Miscibility with	
Water:	Reacts violently
Partition coefficient (n-octanol/water):	Not determined.
Viscosity:	
dynamic:	Not determined.
kinematic:	Not determined.

Solvent content:
Organic solvents: 88,2 %**Solids content:** 11,8 %**9.2 Other information** No further relevant information available.**SECTION 10: Stability and reactivity****10.1 Reactivity**Reacts violently with water.
May form explosive peroxides.
Stable under recommended storage conditions.**10.2 Chemical stability****Thermal decomposition / conditions to be avoided:**

No decomposition if used and stored according to specifications.

10.3 Possibility of hazardous reactionsReacts with strong oxidizing agents
Reacts violently with water
Forms peroxides**10.5 Incompatible materials:**Air
Oxidizing agents
Water/moisture
Heat**10.6 Hazardous decomposition products:**Carbon monoxide and carbon dioxide
Metal oxide
Hydrogen bromide

Trade name **Benzylzinc bromide, 0.5M in THF**

(Contd. of page 3)

SECTION 11: Toxicological information**11.1 Information on toxicological effects**

Acute toxicity: Swallowing will lead to a strong caustic effect on mouth and throat and to the danger of perforation of esophagus and stomach.

LD/LC50 values that are relevant for classification:**109-99-9 Tetrahydrofuran**

Oral	LD50	1650 mg/kg (rat)
Inhalative	LC50/2H	72000 mg/m ³ /2H (rat)

Skin irritation or corrosion:

Causes severe skin burns.

Eye irritation or corrosion:

Causes serious eye damage.

Sensitization:

No sensitizing effect 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.

Additional toxicological information:

To the best of our knowledge the acute and chronic toxicity of this substance is not fully known. The product shows the following dangers according to the calculation method of the General EC Classification Guidelines for Preparations as issued in the latest version:
Corrosive

SECTION 12: Ecological information**12.1 Toxicity****Aquatic toxicity:**

No further relevant information available.

12.2 Persistence and degradability

No further relevant information available.

12.3 Bioaccumulative potential

No further relevant information available.

12.4 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. Water hazard class 1 (Self-assessment): slightly hazardous for water. Do not allow undiluted product or large quantities of it to reach ground water, water bodies or sewage system. Avoid transfer into the environment.

12.5 Results of PBT and vPvB assessment**PBT:**

Not applicable.

vPvB:

Not applicable.

12.6 Other adverse effects

No further relevant information available.

SECTION 13: Disposal considerations**13.1 Waste treatment methods****Recommendation**

Hand over to disposers of hazardous waste. Must be specially treated under adherence to official regulations. Consult state, local or national regulations for proper disposal.

Uncleaned packagings:**Recommendation:**

Disposal must be made according to official regulations.

SECTION 14: Transport information**UN-Number****ADR, IMDG, IATA**

UN3399

14.2 UN proper shipping name**ADR****IMDG, IATA**

3399 ORGANOMETALLIC SUBSTANCE, LIQUID, WATER-REACTIVE, FLAMMABLE
ORGANOMETALLIC SUBSTANCE, LIQUID, WATER-REACTIVE, FLAMMABLE

14.3 Transport hazard class(es)**ADR****Class****Label****IMDG, IATA**

4.3 (WF1) Substances which, in contact with water, emit flammable gases.
4.3+3

**Class****Label**

4.3 Substances which, in contact with water, emit flammable gases.
4.3+3

Packing group**ADR, IMDG, IATA**

II

14.5 Environmental hazards:**Marine pollutant:**

No

14.6 Special precautions for user**Kemler Number:**

Warning: Substances which, in contact with water, emit flammable gases.
323

14.7 Transport in bulk according to Annex II of MARPOL73/78 and the IBC**Code**

Not applicable.

Transport/Additional information:**ADR****Excepted quantities (EQ):**

E2

Limited quantities (LQ)

500 ml

Transport category

0

Tunnel restriction code

D/E

(Contd. on page 5)
DE/E

Safety data sheet
according to 1907/2006/EC, Article 31

Revision: 02.08.2012

Printing date 02.07.2013

Trade name **Benzylzinc bromide, 0.5M in THF**

(Contd. of page 4)

UN "Model Regulation":

UN3399, ORGANOMETALLIC SUBSTANCE, LIQUID, WATER-REACTIVE,
FLAMMABLE, 4.3 (3), II**SECTION 15: Regulatory information****15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture****Australian Inventory of Chemical Substances**

109-99-9 | Tetrahydrofuran

Standard for the Uniform Scheduling of Drugs and Poisons

None of the ingredients is listed.

National regulations**Information about limitation of use:**For use only by technically qualified individuals.
Employment restrictions concerning young persons must be observed.
Not applicable**Classification according to VbF:****Technical instructions (air):**

Class	Share in %
NK	88,2

Water hazard class:

Water hazard class 1 (Self-assessment): slightly hazardous for water.

Other regulations, limitations and prohibitive regulations**ELINCS (European List of Notified Chemical Substances)**

None of the ingredients is listed.

Substances of very high concern (SVHC) according to REACH, Article 57

None of the ingredients are listed.

REACH - Pre-registered substances

109-99-9 | Tetrahydrofuran

15.2 Chemical safety assessment:

A Chemical Safety Assessment has not been carried out.

SECTION 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.

Relevant phrases

H225 Highly flammable liquid and vapour.
H314 Causes severe skin burns and eye damage.
H319 Causes serious eye irritation.
H335 May cause respiratory irritation.
H351 Suspected of causing cancer.

R11 Highly flammable.
R14 Reacts violently with water.
R19 May form explosive peroxides.
R34 Causes burns.
R36/37 Irritating to eyes and respiratory system.
R40 Limited evidence of a carcinogenic effect.

Department issuing data specification sheet:**Abbreviations and acronyms:**

Health, Safety and Environmental Department.
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
IATA: International Air Transport Association
GHS: Globally Harmonized System of Classification and Labelling of Chemicals
VbF: Verordnung über brennbare Flüssigkeiten, Österreich (Ordinance on the storage of combustible liquids, Austria)
LC50: Lethal concentration, 50 percent
LD50: Lethal dose, 50 percent

DE/E