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

Printing date 02.07.2013 *Revision: 21.09.2012*

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifier
Trade name ***4-Bromobenzylzinc bromide, 0.5M in THF***
Stock number: H58662
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 (o) 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.
Xi; Irritant
R37: Irritating to respiratory system.
F; Highly flammable
R11-15: Highly flammable. Contact with water liberates extremely flammable gases.
R19: 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 The product is classified and labelled according to the CLP regulation.
Hazard pictograms GHS02, GHS05, GHS07, GHS08
Signal word Danger
Hazard-determining components of labelling: Tetrahydrofuran
4-Bromobenzylzinc 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: 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	82,2%
CAS: 115055-85-1	4-Bromobenzylzinc bromide C R34; F R15 Water-react. 1, H260; Skin Corr. 1B, H314	17,8%

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Trade name 4-Bromobenzylzinc bromide, 0.5M in THF

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Additional information None known.

SECTION 4: First aid measures

4.1 Description of first aid measures
General information Instantly remove any clothing soiled by the product.
After inhalation Supply fresh air. If required, provide artificial respiration. Keep patient warm. Consult doctor if symptoms persist.
Seek immediate medical advice.
After skin contact Instantly 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 doctor.
After swallowing Seek medical treatment.
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 In case of fire, use sand, carbon dioxide or powdered extinguishing agent. Never use water.
For safety reasons unsuitable extinguishing agents Water.
5.2 Special hazards arising from the substance or mixture 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
Prevention of secondary hazards: Keep away from ignition sources.
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.
Reacts violently with water
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 air.
Protect from heat.
Store away from water.
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 (82,2%)	
AGW (Germany)	150 mg/m³, 50 ppm 2(I);DFG, EU, H, Y
PEL (USA)	590 mg/m³, 200 ppm

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REL (USA)	Short-term value: 735 mg/m³, 250 ppm Long-term value: 590 mg/m³, 200 ppm
TLV (USA)	Short-term value: 295 mg/m³, 100 ppm Long-term value: 147 mg/m³, 50 ppm Skin

Ingredients with biological limit values:

109-99-9 Tetrahydrofuran (82,2%)

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.
Do not inhale dust / smoke / mist.
Avoid contact with the eyes and skin.
Maintain an ergonomically appropriate working environment.
Breathing equipment: Use breathing protection with high concentrations.
Protection of hands: 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.
Material of gloves Impervious gloves
Penetration time of glove material Not determined
Eye protection: Tightly sealed safety glasses.
Full face protection
Body protection: Protective work clothing.

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: 65 °C (THF)
Sublimation temperature / start: Not determined

Flash point: -17 °C (THF)
Inflammability (solid, gaseous) Not determined.
Ignition temperature: 230 °C (THF)
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 % (THF)
Upper: 12,0 Vol % (THF)
Steam pressure at 20 °C: 200 hPa
Density at 20 °C 1,015 g/cm³
Relative density Not determined.
Vapour density Not determined.
Evaporation rate Not determined.
Solubility in / Miscibility with
Water: Contact with water releases flammable gases
Partition coefficient (n-octanol/water): Not determined.
Viscosity:
dynamic: Not determined.
kinematic: Not determined.

Solvent content:
Organic solvents: 82,2 %

Solids content: 17,8 %
9.2 Other information No further relevant information available.

SECTION 10: Stability and reactivity

10.1 Reactivity In contact with water releases flammable gases which may ignite spontaneously.
May form explosive peroxides.
10.2 Chemical stability Stable under recommended storage conditions.
Thermal decomposition / conditions to be avoided: No decomposition if used and stored according to specifications.
10.3 Possibility of hazardous reactions Reacts with strong oxidizing agents
Contact with water releases flammable gases
Forms peroxides
10.5 Incompatible materials: Air
Oxidizing agents
Heat
Water/moisture
10.6 Hazardous decomposition products: Carbon monoxide and carbon dioxide
Hydrogen bromide
Metal oxide

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Additional information: This product may form a precipitate.

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.
The Registry of Toxic Effects of Chemical Substances (RTECS) contains acute toxicity data for components in this product.

LD/LC50 values that are relevant for classification:

109-99-9 Tetrahydrofuran

Oral	LD50	1650 mg/kg (rat)
Inhalative	LC50/2H	72000 mg/m3/2H (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: The Registry of Toxic Effects of Chemical Substances (RTECS) contains mutation data for components in this product.
Carcinogenicity: ACGIH A3: Animal carcinogen: Agent is carcinogenic in experimental animals at a relatively high dose, by route(s) of administration, at site(s), of histologic type(s), or by mechanism(s) not considered relevant to worker exposure. Available epidemiologic studies do not confirm an increased risk of cancer in exposed humans. Available evidence suggests that the agent is not likely to cause cancer in humans except under uncommon or unlikely routes or levels of exposure.
The Registry of Toxic Effects of Chemical Substances (RTECS) contains tumorigenic and/or carcinogenic and/or neoplastic data for this product.
Reproductive toxicity: The Registry of Toxic Effects of Chemical Substances (RTECS) contains reproductive data for components in this product.
Specific target organ system toxicity - repeated exposure: No effects known.
Specific target organ system toxicity - single exposure: May cause respiratory irritation.
Aspiration hazard: No effects known.
Experience with humans: The Registry of Toxic Effects of Chemical Substances (RTECS) contains multiple dose toxicity data for components in this product.
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
Irritant

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 3399 ORGANOMETALLIC SUBSTANCE, LIQUID, WATER-REACTIVE, FLAMMABLE (4-Bromobenzylzinc bromide, TETRAHYDROFURAN)
IMDG, IATA ORGANOMETALLIC SUBSTANCE, LIQUID, WATER-REACTIVE, FLAMMABLE (4-Bromobenzylzinc bromide, TETRAHYDROFURAN)

14.3 Transport hazard class(es)
ADR

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

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

Packing group
ADR, IMDG, IATA II

14.5 Environmental hazards:
Marine pollutant: No

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Trade name *4-Bromobenzylzinc bromide, 0.5M in THF*

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14.6 Special precautions for user Warning: Substances which, in contact with water, emit flammable gases.
Kemler Number: 323
EMS Number: F-G,S-M

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

UN "Model Regulation": UN3399, ORGANOMETALLIC SUBSTANCE, LIQUID, WATER-REACTIVE, FLAMMABLE (4-Bromobenzylzinc bromide, TETRAHYDROFURAN), 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.
Classification according to VbF: A I
Technical instructions (air):

Class	Share in %
NK	82,2

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.
H260 In contact with water releases flammable gases which may ignite spontaneously.
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.
R15 Contact with water liberates extremely flammable gases.
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: Health, Safety and Environmental Department.
Abbreviations and acronyms:
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