

Safety data sheet

according to 1907/2006/EC, Article 31

Revision: 16.11.2011

Printing date 02.07.2013

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

Trade name

4-tert-Butylphenylmagnesium bromide, 0.50 M in 2-MeTHF

Stock number:

H54284

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.



GHS05 corrosion

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

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

Hazard-determining components of labelling:

Hazard statements

Precautionary statements

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

GHS02, GHS05

Danger

4-tert-Butylphenylmagnesium bromide

H225 Highly flammable liquid and vapour.

H314 Causes severe skin burns and eye damage.

P210

Keep away from heat/sparks/open flames/hot surfaces. - No smoking.

P241

Use explosion-proof electrical/ventilating/lighting/equipment.

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: 96-47-9 EINECS: 202-507-4 | 2-Methyltetrahydrofuran | F R11 R19 Flam. Liq. 2, H225 | 87,5% |
| CAS: 63488-10-8 | 4-tert-Butylphenylmagnesium bromide | C R34 R14 Skin Corr. 1B, H314 | 12,5% |

Additional information

None known.

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.

After skin contact

Seek immediate medical advice.

Instantly wash with water and soap and rinse thoroughly.

After eye contact

Seek immediate medical advice.

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.

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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

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.

Prevention of secondary hazards:**6.4 Reference to other sections**

Do not flush with water or aqueous cleansing agents
Keep away from ignition sources.
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.
Store in cool, dry place in tightly closed containers.
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:**

Store in cool location.
Long term storage should be in a refrigerator.

Information about storage in one common storage facility:

Do not store together with acids.
Store away from acid chlorides.
Store away from oxidizing agents.
Store away from water.
Store away from air.

Further information about storage conditions:

Store under dry inert gas.
Protect from humidity and keep away from water.
Store in cool, dry conditions in well sealed containers.
Avoid contact with air / oxygen (formation of peroxide).
Store in a locked cabinet or with access restricted to technical experts or their assistants.
Check container pressure periodically to prevent explosive peroxides.
No further relevant information available.

7.3 Specific end use(s)**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:**

The product does not contain any relevant quantities of materials with critical values that have to be monitored at the workplace.

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

Breathing equipment:**Protection of hands:****Material of gloves****Penetration time of glove material****Eye protection:**(Contd. on page 3)
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Body protection: Protective work clothing.

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SECTION 9: Physical and chemical properties**9.1 Information on basic physical and chemical properties****General Information****Appearance:**

Form: Liquid
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

Flash point: -11 °C (est)
Inflammability (solid, gaseous) Not applicable.
Ignition temperature: Not determined
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: Not determined
Upper: Not determined
Steam pressure: Not determined
Density Not determined
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: 0,0 %

Solids content:

Solids content: 12,5 %

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 reactions

Reacts violently with water
Forms peroxides

10.5 Incompatible materials:

Acids
Air
Acid chlorides
Oxidizing agents
Water/moisture
Carbon monoxide and carbon dioxide
Hydrogen bromide
Metal oxide

10.6 Hazardous decomposition products:**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:**96-47-9 2-Methyltetrahydrofuran**

| | | |
|------------|---------|---------------------|
| Dermal | LD50 | 4500 mg/kg (rabbit) |
| Inhalative | LC50/4H | 6000 ppm/4H (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.

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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**

UN2924

14.2 UN proper shipping name**ADR**

2924 FLAMMABLE LIQUID, CORROSIVE, N.O.S. (4-tert-Butylphenylmagnesium bromide, METHYLTETRAHYDROFURAN)
FLAMMABLE LIQUID, CORROSIVE, N.O.S. (4-tert-Butylphenylmagnesium bromide, METHYLTETRAHYDROFURAN)

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

3 (FC) Flammable liquids.
3+8

**Class****Label**

3 Flammable liquids.
3+8

Packing group**ADR, IMDG, IATA**

II

14.5 Environmental hazards:**Marine pollutant:**

No

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

Warning: Flammable liquids.

EMS Number:338
F-E,S-C**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):****Limited quantities (LQ)****Transport category****Tunnel restriction code**

E2

1L

2

D/E

UN "Model Regulation":

UN2924, FLAMMABLE LIQUID, CORROSIVE, N.O.S. (4-tert-Butylphenylmagnesium bromide, METHYLTETRAHYDROFURAN), 3 (8), II

SECTION 15: Regulatory information**15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture****Australian Inventory of Chemical Substances**

96-47-9 | 2-Methyltetrahydrofuran

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.
A I

Classification according to VbF:

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

Water hazard class:**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

96-47-9 | 2-Methyltetrahydrofuran

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.

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R11 Highly flammable.

R14 Reacts violently with water.

R19 May form explosive peroxides.

R34 Causes burns.

Department issuing data specification sheet:
Abbreviations and acronyms:

Health, Safety and Environmental Department.

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

ICAO: International Civil Aviation Organization

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

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