

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

1.1 Product identifier
Trade name **3-[Cyclopropyl(4-methoxybenzyl)sulfamoyl]benzeneboronic acid**
Stock number: F52845
CAS Number: 913836-07-4

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



GHS07

Skin Irrit. 2 H315 Causes skin irritation.
Eye Irrit. 2 H319 Causes serious eye irritation.
STOT SE 3 H335 May cause respiratory irritation.

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

Xi; Irritant

R36/37/38: Irritating to eyes, respiratory system and skin.

Information concerning particular hazards for human and environment: Not applicable

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 statements

Precautionary statements

The substance is classified and labelled according to the CLP regulation.
GHS07
Warning
H315 Causes skin irritation.
H319 Causes serious eye irritation.
H335 May cause respiratory irritation.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P302+P352 IF ON SKIN: Wash with plenty of soap and water.
P321 Specific treatment (see on this label).
P405 Store locked up.
P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

2.3 Other hazards

Results of PBT and vPvB assessment

PBT: Not applicable.
vPvB: Not applicable.

SECTION 3: Composition/information on ingredients

3.1 Substances

CAS# Designation: 913836-07-4 3-[Cyclopropyl(4-methoxybenzyl)sulfamoyl]benzeneboronic acid

SECTION 4: First aid measures

4.1 Description of first aid measures

After inhalation

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.

After swallowing

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

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

5.2 Special hazards arising from the substance or mixture

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

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

Carbon monoxide and carbon dioxide
Sulphur oxides (SO_x)
Nitrogen oxides (NO_x)
Boron 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

6.2 Environmental precautions:

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

Trade name 3-[Cyclopropyl(4-methoxybenzyl)sulfamoyl]benzeneboronic acid

(Contd. of page 1)

6.3 Methods and material for containment and cleaning up:

Prevention of secondary hazards:

6.4 Reference to other sections

Do not allow product to reach sewage system or water bodies.
Do not allow to enter the ground/soil.

Ensure adequate ventilation.
No special measures required.
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

Keep containers tightly sealed.
Store in cool, dry place in tightly closed containers.
Ensure good ventilation/exhaustion at the workplace.

Information about protection against explosions and fires:

No information known.

7.2 Conditions for safe storage, including any incompatibilities

Storage Requirements to be met by storerooms and containers:

No special requirements.

Information about storage in one common storage facility:

Store away from oxidizing agents.

Further information about storage conditions:

Keep container tightly sealed.
Store in cool, dry conditions in well sealed containers.
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.

Breathing equipment:

Protection of hands:

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.

Material of gloves

Penetration time of glove material

Eye protection:

Impervious gloves

Not determined

Safety glasses

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: Solid.
Colour: Off-white
Smell: Not determined
Odour 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
Inflammability (solid, gaseous) Not determined.
Ignition temperature: Not determined
Decomposition temperature: Not determined
Self-inflammability: Not determined.

Critical values for explosion:

Lower: Not determined
Upper: Not determined

Steam pressure:

Not applicable.

Density Not determined

Relative density Not determined.

Vapour density Not applicable.

Evaporation rate Not applicable.

Solubility in / Miscibility with

Water: Not determined

Partition coefficient (n-octanol/water): Not determined.

Viscosity:

dynamic: Not applicable.

kinematic: Not applicable.

9.2 Other information No further relevant information available.

SECTION 10: Stability and reactivity

10.1 Reactivity

10.2 Chemical stability

Thermal decomposition / conditions to be avoided:

10.3 Possibility of hazardous reactions

10.5 Incompatible materials:

No information known.
Stable under recommended storage conditions.

No decomposition if used and stored according to specifications.

Reacts with strong oxidizing agents

Oxidizing agents

(Contd. on page 3)
DE/E

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

Revision: 09.04.2012

Printing date 02.07.2013

Trade name **3-[Cyclopropyl(4-methoxybenzyl)sulfamoyl]benzeneboronic acid**

10.6 Hazardous decomposition products: Carbon monoxide and carbon dioxide
Boron oxide
Sulphur oxides (SO_x)
Nitrogen oxides (NO_x)

(Contd. of page 2)

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

Acute toxicity: No effects known.
LD/LC50 values that are relevant for classification: No data
Skin irritation or corrosion: Causes skin irritation.
Eye irritation or corrosion: Causes serious eye irritation.
Sensitization: No sensitizing effect known.
Germ cell mutagenicity: No effects known.
Carcinogenicity: EPA-I: Data are inadequate for an assessment of human carcinogenic potential.
Reproductive toxicity: No effects known.
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.
Additional toxicological information: To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.

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, ADN, IMDG, IATA Not applicable

14.2 UN proper shipping name
ADR, ADN, IMDG, IATA Not applicable

14.3 Transport hazard class(es)
ADR, ADN, IMDG, IATA
Class Not applicable

Packing group
ADR, IMDG, IATA Not applicable

14.5 Environmental hazards: Not applicable.

14.6 Special precautions for user Not applicable.

14.7 Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code Not applicable.

UN "Model Regulation": -

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

Australian Inventory of Chemical Substances Substance is not listed.
Standard for the Uniform Scheduling of Drugs and Poisons Substance is not listed.
National regulations
Information about limitation of use: For use only by technically qualified individuals.
Employment restrictions concerning young persons must be observed.
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) Substance is not listed.
Substances of very high concern (SVHC) according to REACH, Article 57 Substance is not listed.
REACH - Pre-registered substances Substance is not listed.
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.

Department issuing data specification sheet: Health, Safety and Environmental Department.

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)

(Contd. on page 4)
DE/E

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

Printing date 02.07.2013

Revision: 09.04.2012

Trade name 3-[Cyclopropyl(4-methoxybenzyl)sulfamoyl]benzeneboronic acid

(Contd. of page 3)
ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
GHS: Globally Harmonized System of Classification and Labelling of Chemicals
CAS: Chemical Abstracts Service (division of the American Chemical Society)
LC50: Lethal concentration, 50 percent
LD50: Lethal dose, 50 percent

DE/E