

SAFETY DATA SHEET

Version 8.7 Revision Date 11/25/2023 Print Date 02/24/2024

SECTION 1: Identification of the substance/mixture and of the company/undertaking **Product identifiers** 1.1 Product name ² 2,4-Dimethoxyphenylmagnesium bromide solution 562025 Product Number : Brand : Aldrich CAS-No. : 138109-49-6 Relevant identified uses of the substance or mixture and uses advised against 1.2 Identified uses : Laboratory chemicals, Synthesis of substances Details of the supplier of the safety data sheet 1.3 Company : Sigma-Aldrich Inc. 3050 SPRUCE ST ST. LOUIS MO 63103 UNITED STATES Telephone : +1 314 771-5765 +1 800 325-5052 Fax : 1.4 **Emergency telephone** Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Flammable liquids (Category 2), H225 Chemicals which, in contact with water, emit flammable gases (Category 2), H261 Acute toxicity, Oral (Category 4), H302 Eye irritation (Category 2A), H319 Carcinogenicity (Category 2), H351 Specific target organ toxicity - single exposure (Category 3), Respiratory system, Central nervous system, H335, H336

For the full text of the H-Statements mentioned in this Section, see Section 16.

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2.2 GHS Label elements, including precautionary statements

Pictogram	
Signal Word	Danger
Hazard Statements	
H225	Highly flammable liquid and vapor.
H261	In contact with water releases flammable gas.
H302	Harmful if swallowed.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
H336	May cause drowsiness or dizziness.
H351	Suspected of causing cancer.
Precautionary Statements	
P201	Obtain special instructions before use.
P202	Do not handle until all safety precautions have been read and understood.
P210	Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P223	Do not allow contact with water.
P231 + P232	Handle under inert gas. Protect from moisture.
P233	Keep container tightly closed.
P240	Ground/bond container and receiving equipment.
P241	Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P261	Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.
P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P271	Use only outdoors or in a well-ventilated area.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P312 + P330	IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P312	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
P335 + P334	Brush off loose particles from skin. Immerse in cool water/ wrap
1555 11554	in wet bandages.
P337 + P313	If eye irritation persists: Get medical advice/ attention.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant
	foam to extinguish.
P402 + P404	Store in a dry place. Store in a closed container.
P403 + P233 P403 + P235	Store in a well-ventilated place. Keep container tightly closed. Store in a well-ventilated place. Keep cool.

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P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal
	plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

May form explosive peroxides.

SECTION 3: Composition/information on ingredients

3.2 Mixtures Formula

Formula	:	C ₈ H ₉ BrMgO ₂
Molecular weight	:	241.36 g/mol

Component		Classification	Concentration
Tetrahydrofuran			
CAS-No. EC-No. Index-No. Registration number	109-99-9 5-53 603-025-00-0 01-2119444314-46- XXXX	Flam. Liq. 2; Acute Tox. 4; Eye Irrit. 2A; Carc. 2; STOT SE 3; H225, H302, H319, H351, H335, H336 Concentration limits: >= 25 %: Eye Irrit. 2, H319; >= 25 %: STOT SE 3, H335;	>= 90 - <= 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. Call in physician.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

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4.3 Indication of any immediate medical attention and special treatment needed No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media Carbon dioxide (CO2) Dry powder

Unsuitable extinguishing media Water Foam

5.2 Special hazards arising from the substance or mixture

Carbon oxides Hydrogen bromide gas Magnesium oxide Combustible. Pay attention to flashback. Vapors are heavier than air and may spread along floors. Risk of dust explosion. May not get in touch with: Water Development of hazardous combustion gases or vapours possible in the event of fire. Forms explosive mixtures with air at ambient temperatures.

5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information

Remove container from danger zone and cool with water. Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains. Risk of explosion.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections For disposal see section 13.

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SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols. Keep workplace dry. Do not allow product to come into contact with water.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed. Keep away from heat and sources of ignition. Never allow product to get in contact with water during storage. **Storage stability**Recommended storage temperature 2 - 8 °C

Handle and store under inert gas. Dry residue is explosive. Test for peroxide formation periodically and before distillation.

Storage class

Storage class (TRGS 510): 4.3: Hazardous materials, which set free flammable gases upon contact with water

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 **Control parameters**

Ingredients with workplace control parameters

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Component	CAS-No.	Value	Control	Basis
			parameters	
Tetrahydrofuran	109-99-9	TWA	50 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Confirmed animal carcinogen with unknown relevance to		
		humans		
		Danger of o	cutaneous absor	ption
		STEL	100 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Confirmed animal carcinogen with unknown relevance to		
		humans		

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Danger of cutaneous absorption		
ST	250 ppm 735 mg/m3	USA. NIOSH Recommended Exposure Limits
TWA	200 ppm 590 mg/m3	USA. NIOSH Recommended Exposure Limits
TWA	200 ppm 590 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
PEL	200 ppm 590 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
STEL	250 ppm 735 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
Tetrahydrofuran	109-99-9	Tetrahydrof uran	2 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift (As soon as possible after exposure ceases)			

8.2 Exposure controls

Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

Personal protective equipment

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

Skin protection

required

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

Recommended Filter type: Filter type ABEK

The entrepeneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

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Control of environmental exposure

Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a)		
۰.,	Appearance	Form: liquid
b)	Odor	No data available
c)	Odor Threshold	No data available
d)	рН	No data available
e)	Melting point/freezing point	No data available
f)	Initial boiling point and boiling range	65.0 - 67.0 °C 149.0 - 152.6 °F
g)	Flash point	-17 °C (1 °F) - closed cup
h)	Evaporation rate	No data available
i)	Flammability (solid, gas)	No data available
j)	Upper/lower flammability or explosive limits	Upper explosion limit: 11.8 %(V) Lower explosion limit: 1.8 %(V)
k)	Vapor pressure	No data available
I)	Vapor density	No data available
m)	Density	0.96 g/cm3 at 25 °C (77 °F)
m)	Density Relative density	0.96 g/cm3 at 25 °C (77 °F) No data available
m) n)		
	Relative density	No data available
n)	Relative density Water solubility Partition coefficient:	No data available No data available
n) o)	Relative density Water solubility Partition coefficient: n-octanol/water Autoignition	No data available No data available No data available
n) o) p)	Relative density Water solubility Partition coefficient: n-octanol/water Autoignition temperature Decomposition	No data available No data available No data available No data available
n) o) p) q)	Relative density Water solubility Partition coefficient: n-octanol/water Autoignition temperature Decomposition temperature	No data available No data available No data available No data available No data available
n) o) p) q) r)	Relative density Water solubility Partition coefficient: n-octanol/water Autoignition temperature Decomposition temperature Viscosity	No data available No data available No data available No data available No data available No data available

9.2 Other safety information No data available

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SECTION 10: Stability and reactivity

10.1 Reactivity

Formation of peroxides possible. Vapors may form explosive mixture with air.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

- 10.3 Possibility of hazardous reactions No data available
- **10.4 Conditions to avoid** Warming. Moisture.
- **10.5 Incompatible materials** Oxidizing agents, Oxygen
- **10.6 Hazardous decomposition products** Peroxides In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Mixture

Acute toxicity

Acute toxicity estimate Oral - 1,651 mg/kg (Calculation method) Symptoms: Possible symptoms:, mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract Acute toxicity estimate Dermal - 2,500 mg/kg (Calculation method)

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

Remarks: Mixture causes serious eye irritation.

Respiratory or skin sensitization

No data available

Germ cell mutagenicity No data available

Carcinogenicity

Evidence of a carcinogenic effect.

- IARC: 2B Group 2B: Possibly carcinogenic to humans (Tetrahydrofuran)
- NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

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OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

Mixture may cause respiratory irritation. Mixture may cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure No data available

Aspiration hazard

No data available

11.2 Additional Information

Central nervous system depression, Cough, chest pain, Difficulty in breathing, Exposure to high airborne concentrations can cause anesthetic effects., To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. Other dangerous properties can not be excluded.

This substance should be handled with particular care.

Handle in accordance with good industrial hygiene and safety practice.

Stomach - Irregularities - Based on Human Evidence

Components

Tetrahydrofuran

Acute toxicity

LD50 Oral - Rat - male and female - 1,650 mg/kg Remarks: (ECHA) Symptoms: Irritation of mucous membranes LC50 Inhalation - Rat - male and female - 6 h - > 14.7 mg/l - vapor (US-EPA) LD50 Dermal - Rat - male and female - > 2,000 mg/kg (OECD Test Guideline 402)

Skin corrosion/irritation

Skin - Rabbit Result: No skin irritation - 72 h (Draize Test) Remarks: Repeated or prolonged exposure may cause skin irritation and dermatitis, due to degreasing properties of the product.

Serious eye damage/eye irritation

Eyes - Rabbit Result: Causes serious eye irritation. Remarks: (IUCLID) Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

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Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse Result: negative (OECD Test Guideline 429)

Germ cell mutagenicity

Test Type: Ames test Test system: S. typhimurium Result: negative Test Type: In vitro mammalian cell gene mutation test Test system: Chinese hamster ovary cells Result: negative Test Type: Chromosome aberration test in vitro Test system: Chinese hamster ovary cells Result: negative Method: OECD Test Guideline 474 Species: Mouse - male and female - Red blood cells (erythrocytes) Result: negative

Carcinogenicity

Suspected of causing cancer.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

Inhalation - May cause respiratory irritation. - Central nervous system Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2) May cause drowsiness or dizziness.

Acute oral toxicity - Irritation of mucous membranes

Specific target organ toxicity - repeated exposure

Aspiration hazard No data available

SECTION 12: Ecological information

12.1 Toxicity

Mixture No data available

- **12.2 Persistence and degradability** No data available
- **12.3 Bioaccumulative potential** No data available
- **12.4 Mobility in soil** No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

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12.6 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

Components

Tetrahydrofuran	
Toxicity to fish	flow-through test LC50 - Pimephales promelas (fathead minnow) - 2,160 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 3,485 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to fish(Chronic toxicity)	flow-through test NOEC - Pimephales promelas (fathead minnow) - 216 mg/l - 33 d Remarks: (ECHA)

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information

DOT (US)

UN number: 3399 Class: 4.3 (3) Packing group: II Proper shipping name: Organometallic substance, liquid, water-reactive, flammable (Tetrahydrofuran, 2,4-Dimethoxyphenylmagnesium bromide) (Tetrahydrofuran, 2,4-Dimethoxyphenylmagnesium bromide) Reportable Quantity (RQ): 1000 lbs Poison Inhalation Hazard: No

IMDG

UN number: 3399 Class: 4.3 (3)

Packing group: II

EMS-No: F-G, S-N

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Proper shipping name: ORGANOMETALLIC SUBSTANCE, LIQUID, WATER-REACTIVE, FLAMMABLE (Tetrahydrofuran, 2,4-Dimethoxyphenylmagnesium bromide) (Tetrahydrofuran, 2,4-Dimethoxyphenylmagnesium bromide)

ΙΑΤΑ

UN number: 3399 Class: 4.3 (3) Packing group: II Proper shipping name: Organometallic substance, liquid, water-reactive, flammable (Tetrahydrofuran, 2,4-Dimethoxyphenylmagnesium bromide) (Tetrahydrofuran, 2,4-Dimethoxyphenylmagnesium bromide)

SECTION 15: Regulatory information

SARA 302 Components

This material does not contain any components with a section 302 EHS TPQ.

SARA 313 Components

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components Tetrahydrofuran	CAS-No. 109-99-9	Revision Date 1993-02-16
Tetrahydrofuran	CAS-No. 109-99-9	Revision Date 1993-02-16
Pennsylvania Right To Know Components Tetrahydrofuran	CAS-No. 109-99-9	Revision Date 1993-02-16
2,4-Dimethoxyphenylmagnesium bromide	138109-49-6	
Tetrahydrofuran	CAS-No. 109-99-9	Revision Date 1993-02-16
New Jersey Right To Know Components Tetrahydrofuran	CAS-No. 109-99-9	Revision Date 1993-02-16
2,4-Dimethoxyphenylmagnesium bromide	138109-49-6	
California Prop. 65 Components , which is/are known to the State of California to	CAS-No.	Revision Date
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SECTION 16: Other information

Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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