

SAFETY DATA SHEET

Version 8.8 Revision Date 11/27/2023 Print Date 09/14/2024

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

1.1 Product identifiers

Product name : 3-Fluoro-4-methoxyphenylmagnesium

bromide

Product Number : 563706 Brand : Aldrich

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

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.

3050 SPRUCE ST ST. LOUIS MO 63103 UNITED STATES

Telephone : +1 314 771-5765 Fax : +1 800 325-5052

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)

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.

2.2 GHS Label elements, including precautionary statements

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Pictogram



Signal Word	Warning
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		Statements
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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.

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.

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. P337 + P313 If eye irritation persists: Get medical advice/ attention.

P403 + P233 Store in a well-ventilated place. Keep container tightly closed.

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 : C₇H₆BrFMgO Molecular weight : 229.33 g/mol

Component		Classification	Concentration
Tetrahydrofuran			
CAS-No.	109-99-9	Flam. Liq. 2; Acute Tox. 4;	>= 70 - < 90
EC-No.	5-53	Eye Irrit. 2A; Carc. 2;	%
Index-No.	603-025-00-0	STOT SE 3; H225, H302,	
Registration	01-2119444314-46-	H319, H351, H335, H336	

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number	XXXX	Concentration limits:
		>= 25 %: Eye Irrit. 2,
		H319; >= 25 %: STOT SE
		3, H335;

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

Consult a physician. Show this material safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. 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

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

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

Use water spray to cool unopened containers.

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4illiPDRC

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SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas.

For personal protection see section 8.

6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wetbrushing and place in container for disposal according to local regulations (see section 13).

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

Advice on protection against fire and explosion

Use explosion-proof equipment. Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

Hygiene measures

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Storage stabilityRecommended storage temperature

2 - 8 °C

Handle and store under inert gas. Air sensitive. Dry residue is explosive.

Storage class

Storage class (TRGS 510): 3: Flammable liquids

7.3 Specific end use(s)

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

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SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Ingredients with workplace control parameters					
Component	CAS-No.	Value	Control	Basis	
			parameters		
Tetrahydrofuran	109-99-9	TWA	50 ppm	USA. ACGIH Threshold Limit	
				Values (TLV)	
	Remarks	Confirmed	irmed animal carcinogen with unknown relevance to ans		
		humans			
		Danger of cutaneous absorption			
		STEL	100 ppm	USA. ACGIH Threshold Limit	
				Values (TLV)	
		Confirmed animal carcinogen with unknown relevance to			
		humans			
		Danger of cutaneous absorption			
		ST	250 ppm	USA. NIOSH Recommended	
			735 mg/m3	Exposure Limits	
		TWA	200 ppm	USA. NIOSH Recommended	
			590 mg/m3	Exposure Limits	
		TWA	200 ppm	USA. Occupational Exposure	
			590 mg/m3	Limits (OSHA) - Table Z-1	
				Limits for Air Contaminants	
		PEL	200 ppm	California permissible exposure	
			590 mg/m3	limits for chemical	
				contaminants (Title 8, Article	
				107)	
		STEL	250 ppm	California permissible exposure	
			735 mg/m3	limits for chemical	
				contaminants (Title 8, Article	
				107)	

Biological occupational exposure limits

biological occupational exposure innits					
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

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.



Personal protective equipment

Eye/face protection

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

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Body Protection

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type AXBEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance Form: liquid

Color: brown

b) Odor No data available

c) Odor Threshold No data available

d) pH No data availablee) Melting No data available

point/freezing point

f) Initial boiling point 65 °C 149 °F - lit. and boiling range

g) Flash point < -17 °C (< 1 °F) - closed cup

h) Evaporation rate No data available

i) Flammability (solid, No data available gas)

j) Upper/lower

explosive limits

Upper/lower No data available flammability or



k) Vapor pressure
No data available
No data available
No data available
O.964 g/cm3
Relative density
No data available

p) Autoignition No data available

temperature q) Decomposition

No data available

temperature

r) Viscosity No data available

s) Explosive properties Not classified as explosive.

t) Oxidizing properties none

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

No data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

Vapors may form explosive mixture with air.

10.4 Conditions to avoid

Heat, flames and sparks. Extremes of temperature and direct sunlight.

10.5 Incompatible materials

Oxidizing agents, Oxygen

10.6 Hazardous decomposition products

In the event of fire: see section 5



SECTION 11: Toxicological information

11.1 Information on toxicological effects

Mixture

Acute toxicity

Oral: No data available Inhalation: No data available Dermal: No data available

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

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.

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

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., spasm, inflammation and edema of the larynx, spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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)

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

12.6 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

Components

Tetrahydrofuran

flow-through test LC50 - Pimephales promelas (fathead Toxicity to fish

minnow) - 2,160 mg/l - 96 h (OECD Test Guideline 203)

Toxicity to daphnia

static test EC50 - Daphnia magna (Water flea) - 3,485 mg/l -

and other aquatic

48 h invertebrates (OECD Test Guideline 202)

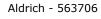
Toxicity to

flow-through test NOEC - Pimephales promelas (fathead

fish(Chronic toxicity)

minnow) - 216 mg/l - 33 d

Remarks: (ECHA)



SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

DOT (US)

UN number: 2924 Class: 3 (8) Packing group: II

Proper shipping name: Flammable liquids, corrosive, n.o.s. (3-Fluoro-4methoxyphenylmagnesium bromide, Tetrahydrofuran) (3-Fluoro-4-methoxyphenylmagnesium bromide, Tetrahydrofuran)

Reportable Quantity (RQ): 1135 lbs Poison Inhalation Hazard: No

IMDG

UN number: 2924 Class: 3 (8) Packing group: II EMS-No: F-E, S-C Proper shipping name: FLAMMABLE LIQUID, CORROSIVE, N.O.S. (3-Fluoro-4methoxyphenylmagnesium bromide, Tetrahydrofuran) (3-Fluoro-4methoxyphenylmagnesium bromide, Tetrahydrofuran)

IATA

UN number: 2924 Class: 3 (8) Packing group: II Proper shipping name: Flammable liquid, corrosive, n.o.s. (3-Fluoro-4methoxyphenylmagnesium bromide, Tetrahydrofuran) (3-Fluoro-4methoxyphenylmagnesium bromide, Tetrahydrofuran)

SECTION 15: Regulatory information

SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

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

Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

CAS-No. Revision Date

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Tetrahydrofuran	109-99-9	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
3-Fluoro-4-methoxyphenylmagnesium bromide	112780-67-3	
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
3-Fluoro-4-methoxyphenylmagnesium bromide	112780-67-3	
California Prop. 65 Components , which is/are known to the State of California to cause cancer. For more information go to www.P65Warnings.ca.gov.Tetrahydrofuran	CAS-No. 109-99-9	Revision Date 2021-12-31

SECTION 16: Other information

Further information

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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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