

Safety Data Sheet

#90027186 · Full 16-section SDS

According to Regulation (EC) No 1907/2006

According to Regulation (EC) No 2020/878

PRODUCT	CAS NUMBER	FORMULA	VERSION	REVISION DATE
Phenylmagnesium bromide 1M in THF	100-58-3	C6H5MgBr	10	13 Oct 2026

SECTION 1

Identification

1.1 Product identifier

Product name	Phenylmagnesium bromide 1M in THF
CAS number	100-58-3
EC / EINECS number	202-867-2
UFI code	7F5W-FEWE-FC8P-CHA4
Chemical formula	C6H5MgBr
Molecular weight	181.31
SMILES	<chem>C1=CC=[C-]C=C1.[Mg+2].[Br-]</chem>

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

Research and development, laboratory chemicals, manufacture of substances; not suitable for human consumption or veterinary purposes.

1.3 Details of the supplier of the safety data sheet

Molekula Limited
1 Millennium Way, Newton Aycliffe
Durham, DL5 6JW, United Kingdom
info@molekula.com · +44 (0) 3302 000333

1.4 Emergency telephone number

0344 892 0111 — National Poisons Information Service (NPIS) (United Kingdom — for healthcare professionals (via TOXBASE))

SECTION 2

Hazard identification

2.1 Classification of the substance or mixture

Flam. Liq. 2, H225

Water-react. 1, H260

Acute Tox. 4 (oral), H302

Skin Corr. 1B, H314

STOT SE 3 (respiratory tract irritation), H335

STOT SE 3 (narcosis), H336

Carc. 2, H351

2.2 Label elements



DANGER

CODE	HAZARD STATEMENT
------	------------------

EUH014	Reacts violently with water
---------------	-----------------------------

EUH019	May form explosive peroxides
---------------	------------------------------

H225	Highly flammable liquid and vapour
-------------	------------------------------------

H260	In contact with water releases flammable gases which may ignite spontaneously
-------------	---

H314 (sub cat. 1B)	Causes severe skin burns and eye damage
---------------------------	---

H336	May cause drowsiness or dizziness
-------------	-----------------------------------

H351	Suspected of causing cancer
-------------	-----------------------------

CODE	PRECAUTIONARY STATEMENT
------	-------------------------

P210	Keep away from heat/sparks/open flames/hot surfaces - No smoking
-------------	--

P223	Keep away from any possible contact with water, because of violent reaction and possible flash fire
-------------	---

P260	Do not breathe dust/fume/gas/mist/vapours/spray
-------------	---

P280	Wear protective gloves/protective clothing/eye protection/face protection
-------------	---

P301+310	IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician
-----------------	--

P308+313	IF exposed or concerned: Get medical advice/attention
-----------------	---

2.3 Other hazards

No data available.

SECTION 3

Composition / information on ingredients

3.2 Mixtures

COMPONENT 1

Name	Phenylmagnesium bromide
CAS number	100-58-3
EC number	202-867-2
Concentration	10-20%
Classification according to Regulation (EC) No 1272/2008	Water-react. 1; H260 Skin Corr. 1; H314
Hazard statements	H260, H314

COMPONENT 2

Name	Tetrahydrofuran
CAS number	109-99-9
EC number	203-726-8
Concentration	80-90%
Classification according to Regulation (EC) No 1272/2008	Flam. Liq. 2; H225 Acute Tox. 4; H302 Eye Irrit. 2; H319 STOT SE 3; H335 STOT SE 3; H336 Carc. 2; H351
Hazard statements	EUH019, H225, H302, H319, H335, H336, H351
Acute toxicity estimate (ATE)	STOT SE 3; H335: C ≥ 25 % Eye Irrit.2; H319: C ≥ 25 %;

SECTION 4**First-aid measures****4.1 Description of first aid measures**

Inhalation	Remove person to fresh air and keep comfortable for breathing; immediately call a poison center/doctor; give artificial respiration if breathing stops and oxygen if breathing is difficult.
Skin contact	Take off immediately all contaminated clothing, rinse skin with water or shower, and immediately call a poison center/doctor.
Eye contact	Remove contact lenses if present, rinse eyes with water for at least 15 minutes and seek medical attention.
Ingestion	Give water to drink (two glasses at most), seek medical advice immediately; induce vomiting only in exceptional cases if medical care is unavailable within one hour and the person is fully conscious; administer activated charcoal; do not attempt to neutralise.

Get medical attention if any discomfort continues. Show this Safety Data Sheet (SDS) to medical personnel. First aiders/ medical personnel need to protect themselves.

4.2 Most important symptoms and effects, both acute and delayed

Not applicable

4.3 Indication of any immediate medical attention and special treatment needed

Treat symptomatically; immediately call a poison center/doctor.

SECTION 5

Fire-fighting measures

5.1 Extinguishing media

Suitable extinguishing media Carbon dioxide or dry powder.

Unsuitable extinguishing media Water; foam.

5.2 Special hazards arising from the substance or mixture

Highly flammable and corrosive, reacts violently with water; may release CO, CO₂, hydrogen bromide and magnesium oxide; containers may burst when heated; vapours are heavier than air, may form explosive mixtures and flash back.

5.3 Advice for firefighters

Evacuate area, avoid breathing fumes, wear suitable protective equipment and keep a safe distance; cool exposed containers with water spray and remove them if safe to do so.

SECTION 6

Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Avoid inhaling vapours and contact with skin and eyes, wear PPE (see section 8), ensure adequate ventilation, remove ignition sources and prevent static discharges.

6.2 Environmental precautions

Avoid discharge into drains, water courses or onto the ground; risk of explosion.

6.3 Methods and material for containment and cleaning up

Collect with absorbent, non-combustible material into suitable containers using spark-proof tools and explosion-proof equipment; remove ignition sources.

6.4 Reference to other sections

For specific precautions, see Section 8 and Section 13.

SECTION 7

Handling & storage

7.1 Precautions for safe handling

Keep away from heat, sparks, open flames and ignition sources; prevent static discharge; use spark-proof tools and explosion-proof equipment; work under hood; wear protective clothing, gloves, eye and face protection; avoid contact with skin and eyes, ingestion and inhalation.

7.2 Conditions for safe storage, including any incompatibilities

Storage temperature Ambient

Conditions for safe storage (incompatibilities) Store at ambient temperature in a dry place in a closed container under inert gas; do not allow contact with water; test periodically for peroxides; dry residue is explosive; storage class 4.3 (water reactive).

7.3 Specific end use(s)

See Section 1.2.

SECTION 8

Exposure controls / personal protection

8.1 Control parameters

Occupational exposure limits (OEL / WEL) Tetrahydrofuran (CAS 109-99-9): short-term exposure limit 100 ppm / 300 mg/m³.

DNEC/PNEC data THF DNEL (workers): dermal chronic systemic 12.6 mg/kg bw/day; inhalation acute local 300 mg/m³, acute systemic 96 mg/m³, chronic local 150 mg/m³, chronic systemic 3.5 mg/m³.

THF PNEC: freshwater 4.32 mg/l, marine water 0.432 mg/l, freshwater sediment 23.3 mg/kg, marine sediment 2.33 mg/kg, intermittent releases 21.6 mg/l, STP 4.6 mg/l, soil 2.13 mg/kg.

8.2 Exposure controls

Eye / face protection Safety glasses
Wear eye/face protection as recommended. All eye/face protection should comply with EN ISO 16321-1:2022.

Skin / hand protection Protective gloves.

Respiratory protection Self-contained breathing apparatus
Keep self-contained breathing apparatus readily available for emergency use. Provide adequate ventilation. If ventilation is insufficient, suitable respiratory protection must be provided. Respiratory equipment: Reusable Air-Purifying Respirator (APR). Filter type: ABEK. Standard: EN 14387.

Other protection Wash skin thoroughly after handling.

Environmental exposure controls Avoid discharge into drains.

SECTION 9

Physical & chemical properties

9.1 Information on basic physical and chemical properties

Appearance / physical state Liquid

DERIVED FROM: LITERATURE

Colour Dark brown

DERIVED FROM: LITERATURE

Odour	Not known DERIVED FROM: LITERATURE
Melting / freezing point	<i>Not applicable</i>
Boiling point	69°C DERIVED FROM: LITERATURE
Flammability	Flammable liquid and vapour. DERIVED FROM: LITERATURE
Lower and upper explosion limit	<i>No data available</i>
Flash point	-17 °C DERIVED FROM: LITERATURE
Auto-ignition temperature	<i>Not applicable</i>
Decomposition temperature	<i>No data available</i>
pH	<i>Not applicable</i>
Acidity	Base DERIVED FROM: LITERATURE
Kinematic viscosity	<i>No data available</i>
Solubility	Reacts violently with water. DERIVED FROM: LITERATURE
Partition coefficient n-octanol/water (log value)	<i>Not applicable</i>
Vapour pressure	<i>Not applicable</i>
Density (g/mL)	1.004 g/mL DERIVED FROM: LITERATURE
Relative vapour density	<i>No data available</i>
Particle characteristics	<i>No data available</i>

9.2 Other information

No data available

SECTION 10

Stability & reactivity

10.1 Reactivity

Risk of explosion if heated under confinement; vapour/air mixtures explosive at intense warming; peroxide formation possible.

10.2 Chemical stability

Stable under normal temperature and prescribed storage conditions; air and moisture sensitive.

10.3 Possibility of hazardous reactions

Reacts violently with water.

10.4 Conditions to avoid

Heat, sparks, flames. Avoid moisture

10.5 Incompatible materials

Acids, alcohols, strong oxidising agents, water.

10.6 Hazardous decomposition products

See section 5

SECTION 11

Toxicological information

11.1 Information on hazard classes as defined in Regulation (EC) No 1272/2008

Acute toxicity (LD50 / LC50)	Classification criteria not met; THF: LD50 oral rat 1650 mg/kg, LD50 dermal rabbit >2000 mg/kg, LC50 inhalation rat 14.7 mg/l vapour (6 h).
Skin corrosion / irritation	Classification criteria not met; THF: no skin irritation (rabbit, 72 h).
Eye corrosion / irritation	Classification criteria not met; THF: causes serious eye irritation (rabbit).
Respiratory / skin sensitisation	Classification criteria not met; THF: negative (mouse LLNA).
Carcinogenicity	Classification criteria not met; THF: suspected of causing cancer.
Mutagenicity	Classification criteria not met; THF negative in Ames, CHO gene mutation, chromosome aberration and mouse micronucleus tests.
Reproductive toxicity	Based on available data, the classification criteria are not met.
STOT (single / repeated exposure)	Classification criteria not met; THF may cause respiratory irritation and drowsiness or dizziness (CNS); repeated exposure criteria not met.
Aspiration hazard	Based on available data, the classification criteria are not met.

11.2 Information on other hazards

Not classified

SECTION 12

Ecological information

12.1 Toxicity

Tetrahydrofuran: LC50 2160 mg/l (96 h, Pimephales promelas); EC50 3485 mg/l (48 h, Daphnia magna); chronic NOEC 216 mg/l (33 days, Pimephales promelas).

12.2 Persistence and degradability

Tetrahydrofuran: 39% aerobic degradation in 28 days - not readily biodegradable.

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

No data available

12.6 Endocrine disrupting properties

See Section 11.2.

12.7 Other adverse effects

No data available

SECTION 13

Disposal considerations

13.1 Waste treatment methods

Dispose of contents/container in accordance with local regulations.

SECTION 14

Transport information

14.1 UN number or ID number

UN3399

14.2 UN proper shipping name

ORGANOMETALLIC SUBSTANCE, LIQUID, WATER-REACTIVE, FLAMMABLE

14.3 Transport hazard class(es)

3(8)



14.4 Packing group

I

14.5 Environmental hazards

Not applicable

14.6 Special precautions for user

Special precautions for user Tunnel restriction code B/E; transport category 0; IMDG EmS F-G, S-N; ADR/RID classification code WF1, hazard identification number X323.

Transport category 0

Tunnel code (B/E)

Packing instruction (ADR) P402

Packing instruction (IMDG) P402

14.7 Maritime transport in bulk according to IMO instruments

No data available

SECTION 15

Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

Substance-specific regulations (e.g. licences)

National Regulations:

-Seveso III: Directive 2012/18/EU of the European Parliament and of the Council on the control of major-accident hazards involving dangerous substances

Other regulations, limitations and legal regulations:

-Directive 94/33/EC- The protection of young people at work.

REACH code

Y110

ECHA notification

Not applicable

15.2 Chemical safety assessment

Not applicable

SECTION 16

Other information

Revision notes / other information

Version 2.0, issued 2025-10-13, replaces SDS dated 2022-07-04; includes full text of hazard classes and H/EUH phrases (H225, H260, H302, H314, H319, H335, H336, H351, EUH014, EUH019).

This Safety Data Sheet was generated automatically from the data Molekula holds against this product, in the 16-section GHS/CLP format. Fields shown as "No data available" carry no recorded value; fields shown as "Not applicable" were assessed as not relevant to this substance. For queries, contact Molekula at info@molekula.com.