Chemical Safety Data Sheet MSDS / SDS

2-Phenylbutyryl chloride

Revision Date:2025-07-19 Revision Number:1

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

Product identifier

: 2-Phenylbutyryl chloride						
: CB8285593						
: 36854-57-6						
: 253-241-0						
: 2-phenylbutanoyl chloride,2-Phenylbutyric chloride						
Relevant identified uses of the substance or mixture and uses advised against						
: For R&D use only. Not for medicinal, household or other use.						
: none						
: Chemicalbook						
: Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing						
: 010-86108875						

SECTION 2: Hazards identification

GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Danger

Precautionary statements

P501 Dispose of contents/container to.....

P406 Store in corrosive resistant/... container with a resistant inner liner.

P405 Store locked up.

P390 Absorb spillage to prevent material damage.

P310 Immediately call a POISON CENTER or doctor/physician.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continuerinsing.

P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.

P301+P330+P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

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

P264 Wash skin thouroughly after handling.

P264 Wash hands thoroughly after handling.

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

P234 Keep only in original container.

Hazard statements

H318 Causes serious eye damage

H314 Causes severe skin burns and eye damage

H290 May be corrosive to metals

SECTION 3: Composition/information on ingredients

Substance

Product name	: 2-Phenylbutyryl chloride
Synonyms	: 2-phenylbutanoyl chloride,2-Phenylbutyric chloride
CAS	: 36854-57-6
EC number	: 253-241-0
MF	: C10H11CIO
MW	: 182.65

SECTION 4: First aid measures

Description of first aid measures

General advice

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

If inhaled

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

In case of skin contact

Take off contaminated clothing and shoes immediately. 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.

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

Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

Extinguishing media

Suitable extinguishing media

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

Special hazards arising from the substance or mixture

Carbon oxides, Hydrogen chloride gas Carbon oxides, Hydrogen chloride gas

Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

Further information

No data available

NFPA 704

3		0
HEALTH	3	Short exposure could cause serious temporary or moderate residual injury (e.g. <u>liquid hydrogen, sulfuric acid</u> , <u>calcium</u> <u>hypochlorite</u> , hexafluorosilicic acid)
FIRE	1	Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. <u>mineral oil</u> , ammonia)
REACT	0	Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, N2)
SPEC. HAZ.		

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. For personal protection see section 8.

Environmental precautions

Do not let product enter drains.

Methods and materials for containment and cleaning up

Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

Reference to other sections

SECTION 7: Handling and storage

Precautions for safe handling

Avoid inhalation of vapor or mist.

Normal measures for preventive fire protection. For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

Store in cool place. 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.

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

control parameter

Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

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

Tightly fitting safety goggles. Faceshield (8-inch minimum). 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.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it. Body Protection

Complete suit protecting against chemicals, 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 ABEK (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

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance	colorless clear, liquid
Odour	No data available
Odour Threshold	No data available
рН	No data available
Melting point/freezing point	178-180 °C
Initial boiling point and boiling range	122 - 125 °C at 27 hPa - lit.
Flash point	98 °C - closed cup
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive	No data available
limits	
Vapour pressure	No data available
Vapour density	No data available
Relative density	1,093 g/mL at 25 °C
Water solubility	No data available
Partition coefficient: n-octanol/water	No data available
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	No data available
Explosive properties	No data available
Oxidizing properties	No data available

Other safety information

No data available

SECTION 10: Stability and reactivity

Reactivity

No data available

Chemical stability

Stable under recommended storage conditions.

Possibility of hazardous reactions

No data available

Conditions to avoid

No data available

Incompatible materials

Strong oxidizing agents

Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Hydrogen chloride gas Hazardous decomposition products formed under fire conditions. - Carbon oxides, Hydrogen chloride gas Other decomposition products - No data available In the event of fire: see section 5

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity
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
ARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human
carcinogen by IARC.
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
Additional Information
RTECS: Not available
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,
aryngitis, Shortness of breath, Headache, Nausea, Vomiting, To the best of our knowledge, the chemical, physical, and toxicological
properties have not been thoroughly investigated.

Toxicity

No data available

Persistence and degradability

No data available

Bioaccumulative potential

No data available

Mobility in soil

No data available

Results of PBT and vPvB assessment

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

Other adverse effects

No data available

SECTION 13: Disposal considerations

Waste treatment methods

Product

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

UN number

ADR/RID: 3265 IMDG: 3265 IATA: 3265

UN proper shipping name

ADR/RID: CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S. (2-Phenylbutyryl chloride) IMDG: CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S.

(2-Phenylbutyryl chloride)

IATA: Corrosive liquid, acidic, organic, n.o.s. (2-Phenylbutyryl chloride)

Transport hazard class(es)

ADR/RID: 8 IMDG: 8 IATA: 8

Packaging group

ADR/RID: II IMDG: II IATA: II

Environmental hazards

ADR/RID: no IMDG Marine pollutant: no IATA: no

Special precautions for user

No data available

SECTION 15: Regulatory information

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

Regulations on the Safety Management of Hazardous Chemicals China Catalog of Hazardous chemicals 2015:Not Listed. website: https://www.mem.gov.cn/ Measures for Environmental Management of New Chemical Substances United States Toxic Substances Control Act (TSCA) Inventory:Not Listed. website: https://www.epa.gov/ Philippines Inventory of Chemicals and Chemical Substances (PICCS):Not Listed. website: https://emb.gov.ph/ New Zealand Inventory of Chemicals (NZIoC):Not Listed. website: https://www.epa.govt.nz/ Korea Existing Chemicals List (KECL):Not Listed. website: http://ncis.nier.go.kr Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Not Listed. website: https://www.mee.gov.cn/ Vietnam National Chemical Inventory:Listed. website: https://chemicaldata.gov.vn/ European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: https://echa.europa.eu/ EC Inventory:Listed.

SECTION 16: Other information

Abbreviations and acronyms

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

- CAS: Chemical Abstracts Service
- EC50: Effective Concentration 50%
- IATA: International Air Transportation Association
- IMDG: International Maritime Dangerous Goods
- LC50: Lethal Concentration 50%
- LD50: Lethal Dose 50%
- RID: Regulation concerning the International Carriage of Dangerous Goods by Rail
- STEL: Short term exposure limit
- TWA: Time Weighted Average

References

- [1] CAMEO Chemicals, website: http://cameochemicals.noaa.gov/search/simple
- [2] ChemlDplus, website: http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp
- [3] ECHA European Chemicals Agency, website: https://echa.europa.eu/
- [4] eChemPortal The Global Portal to Information on Chemical Substances by OECD, website:

http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

- [5] ERG Emergency Response Guidebook by U.S. Department of Transportation, website: http://www.phmsa.dot.gov/hazmat/library/erg
- [6] Germany GESTIS-database on hazard substance, website: http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp
- [7] HSDB Hazardous Substances Data Bank, website: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm
- [8] IARC International Agency for Research on Cancer, website: http://www.iarc.fr/
- [9] IPCS The International Chemical Safety Cards (ICSC), website: http://www.ilo.org/dyn/icsc/showcard.home
- [10] Sigma-Aldrich, website: https://www.sigmaaldrich.com/

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.