Chemical Safety Data Sheet MSDS / SDS

Hydrocinnamoyl chloride

Revision Date:2025-02-01 Revision Number:1

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

Product identifier

Product name	: Hydrocinnamoyl chloride				
CBnumber	: CB7731088				
CAS	: 645-45-4				
EINECS Number	: 211-443-6				
Synonyms	: 3-phenylpropanoyl chloride, Hydrocinnamoyl chloride				
Relevant identified uses of the substance or mixture and uses advised against					
Relevant identified uses	: For R&D use only. Not for medicinal, household or other use.				
Uses advised against	: none				
Company Identification					
Company	: Chemicalbook				
Address	: Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing				
Telephone	: 010-86108875				

SECTION 2: Hazards identification

GHS Label elements, including precautionary statements

Symbol(GHS)

Signal word

Danger

Precautionary statements

P405 Store locked up.

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.

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

Hazard statements

H332 Harmful if inhaled

SECTION 3: Composition/information on ingredients

Substance

Product name	: Hydrocinnamoyl chloride
Synonyms	: 3-phenylpropanoyl chloride, Hydrocinnamoyl chloride
CAS	: 645-45-4
EC number	: 211-443-6
MF	: C9H9CIO
MW	: 168.62

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. Take victim immediately to hospital. 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 Combustible.

Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

Further information

No data available

NFPA 704



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. mineral oil, ammonia)
REACT	2	Undergoes violent chemical change at elevated temperatures and pressures, reacts violently with water, or may form explosive mixtures with water (e.g. white phosphorus, <u>potassium</u> , <u>sodium</u>)
SPEC. HAZ.	₩	

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

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

Environmental precautions

Prevent further leakage or spillage if safe to do so. 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

For disposal see section 13.

Precautions for safe handling

Advice on safe handling

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

Hygiene measures

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

Storage conditions

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.

Moisture sensitive.

Storage class

Storage class (TRGS 510): 6.1D: Non-combustible, acute toxic Cat.3 / toxic hazardous materials or hazardous materials causing chronic effects

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

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. Full contact

Material: Fluorinated rubber Minimum layer thickness: 0,7 mm Break through time: 480 min

Material tested: Vitoject? (KCL 890 / Aldrich Z677698, Size M) Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0,4 mm Break through time: 30 min

Material tested:Camatril? (KCL 730 / Aldrich Z677442, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

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

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

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance	yellow clear, liquid
Odour	No data available
Odour Threshold	No data available
рН	No data available
Melting point/freezing point	Melting point/range: -75 °C - lit.
Initial boiling point and boiling range	107 °C at 15 hPa - lit.
Flash point	227 °F
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	1,135 g/cm3 at 25 °C - lit. No data available
Water solubility	No data available
Partition coefficient: n-octanol/water	No data available
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: 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

Water, Alcohols, Oxidizing agents, Strong bases

Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity Oral LC50 Inhalation - 4 h - 11 mg/l LC50 Inhalation - Rat - 4 h - 2.750 mg/m3 Remarks: Sense Organs and Special Senses (Nose, Eye, Ear, and Taste):Eye:Other. Lungs, Thorax, or Respiration:Other changes. Skin and Appendages: Other: Hair. Dermal 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 No data available

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

SECTION 12: Ecological information

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

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

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.

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. (3-Phenylpropionyl chloride) IMDG: CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S. (3-Phenylpropionyl chloride) IATA: Corrosive liquid, acidic, organic, n.o.s. (3-Phenylpropionyl 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 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/ United States Toxic Substances Control Act (TSCA) Inventory:Listed. website: https://www.epa.gov/ Philippines Inventory of Chemicals and Chemical Substances (PICCS):Listed. website: https://emb.gov.ph/ New Zealand Inventory of Chemicals (NZIoC):Listed. website: https://www.epa.govt.nz/ 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.