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SAFETY DATA SHEET according to Regulation (EC) No. 1907/2006

Version 6.2 Revision Date 02.10.2022 Print Date 08.05.2024 GENERIC EU MSDS - NO COUNTRY SPECIFIC DATA - NO OEL DATA

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

1.1	Product identifiers Product name	:	5-Methyl-1-phenyl-3-hexanone		
	Product Number Brand REACH No.	:	S411000 Aldrich A registration number is not available for this substance as the substance or its uses are exempted from registration, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.		
	CAS-No.	:	78987-82-3		
1.2	Relevant identified uses of the substance or mixture and uses advised against				
	Identified uses	:	Laboratory chemicals, Manufacture of substances		
1.3	Details of the supplier of the safety data sheet				
	Company	:	Merck Life Science S.r.I. Via Monte Rosa 93 I-20149 MILANO		
1.4	Telephone Fax E-mail address Emergency telephone		+39 02 3341 7340 +39 02 3801 0737 serviziotecnico@merckgroup.com		
1.7	Emergency Phone #	:	800-789-767 (CHEMTREC Italia) +39-02-4555-7031 (CHEMTREC chiamate internazionali) +39 02-6610-1029 (Centro Antiveleni Niguarda Ca' Granda - Milano)		

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008 Acute toxicity, Oral (Category 4), H302

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

2.2 Label elements

Labelling according Regulation (EC) No 1272/2008

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Pictogram	
Signal Word	Warning
Hazard statement(s) H302	Harmful if swallowed.
Precautionary statement(s)	none
Supplemental Hazard Statements	none

2.3 Other hazards - none

SECTION 3: Composition/information on ingredients

3.1 Substances

Formula	
Molecular weight	
CAS-No.	

: C13H18O : 190,29 g/mol : 78987-82-3

Component		Classification	Concentration			
5-Methyl-1-phenyl-3-hexanone						
CAS-No.	78987-82-3	Acute Tox. 4; H302	<= 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

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

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

In case of eye contact

Flush eyes with water as a precaution.

If swallowed

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

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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

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 No data available

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Avoid breathing dust. 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. Discharge into the environment must be avoided.

- **6.3 Methods and materials for containment and cleaning up** Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.
- **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 formation of dust and aerosols.

Advice on protection against fire and explosion

Provide appropriate exhaust ventilation at places where dust is formed.Normal measures for preventive fire protection.

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

Store in cool place. Keep container tightly closed in a dry and well-ventilated place.

Storage class

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Storage class (TRGS 510): 13: Non Combustible Solids

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

8.2 Exposure controls

Personal protective equipment

Eye/face protection

Safety glasses with side-shields conforming to EN166 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

For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator.For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges. 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. Discharge into the environment must be avoided.

SECTION 9: Physical and chemical properties 9.1 Information on basic physical and chemical properties

- a) Physical state solid
- b) Color No data available
- c) Odor No data available
- d) Melting No data available point/freezing point
- e) Initial boiling point No data available and boiling range

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f)	Flammability (solid, gas)	No data available
g)	Upper/lower flammability or explosive limits	No data available
h)	Flash point	No data available
i)	Autoignition temperature	No data available
j)	Decomposition temperature	No data available
k)	рН	No data available
I)	Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
m)	Water solubility	No data available
n)	Partition coefficient: n-octanol/water	log Pow: 3,583
o)	Vapor pressure	No data available
p)	Density	No data available
	Relative density	No data available
q)	Relative vapor density	No data available
r)	Particle characteristics	No data available

- s) Explosive properties No data available
- t) Oxidizing properties No data available
- 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** No data available
- **10.4 Conditions to avoid** No data available
- **10.5 Incompatible materials** Strong oxidizing agents
- **10.6 Hazardous decomposition products** In the event of fire: see section 5

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SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

Acute toxicity estimate Oral - 500 mg/kg (Calculation method) Oral: No data available LD50 Oral - 500,1 mg/kg Inhalation: No data available Dermal: No data available

Skin corrosion/irritation

Remarks: No data available

Serious eye damage/eye irritation Remarks: 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

11.2 Additional Information

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

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish

LC50 - Pimephales promelas (fathead minnow) - 30,5 mg/l - 96,0 h Remarks: The preceding data, or interpretation of data, was determined using Quantitative Structure Activity Relationship (QSAR) modeling.

No data available

12.2 Persistence and degradability

No data available

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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

Harmful to aquatic life. No data available

SECTION 13: Disposal considerations

13.1 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. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information					
14.1 UN number ADR/RID: -	IMDG:	-	IATA: -		
IMDG: Not	hipping name t dangerous goods t dangerous goods t dangerous goods				
14.3 Transport ha ADR/RID: -	zard class(es) IMDG:	-	IATA: -		
14.4 Packaging gr ADR/RID: -	r oup IMDG:	-	IATA: -		
14.5 Environment ADR/RID: no		Marine pollutant: no	IATA: no		
14.6 Special preca	autions for user				

tero special precautions for us

Further information

Not classified as dangerous in the meaning of transport regulations.

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SECTION 15: Regulatory information

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

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

International Chemical Weapons Convention (CWC) Schedules of Toxic Chemicals and Precursors	:
Restrictions on the marketing and use of certain dangerous substances and preparations	:
Regulation (EC) No 649/2012 of the European Parliament and the Council concerning the export and import of dangerous chemicals	:
Candidate List of Substances of Very High Concern for Authorisation	:

15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out

SECTION 16: Other information

Full text of H-Statements referred to under sections 2 and 3.

H302 Harmful if swallowed.

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Full text of other abbreviations

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways; ADR - Agreement concerning the International Carriage of Dangerous Goods by Road; AIIC - Australian Inventory of Industrial Chemicals; ASTM -American Society for the Testing of Materials; bw - Body weight; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; ELx - Loading rate associated with x% response; EmS -Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx -Concentration associated with x% growth rate response; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; n.o.s. Not Otherwise Specified; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NZIOC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RID - Regulations concerning the International Carriage of Dangerous Goods by Rail; SADT - Self-Accelerating Decomposition Temperature; SDS Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

Further information

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The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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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