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Acetophenone ≥98 %, for synthesis

article number: **0986** Version: **GHS 3.0 en** Replaces version of: 2022-09-21 Version: (GHS 2)

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

1.1 Product identifier

Identification of the substance

Article number

CAS number

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98-86-2

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

Relevant identified uses:

Uses advised against:

Laboratory and analytical use Laboratory chemical

Do not use for private purposes (household). Food, drink and animal feedingstuffs.

1.3 Details of the supplier of the safety data sheet

Carl Roth GmbH + Co. KG Schoemperlenstr. 3-5 D-76185 Karlsruhe Germany

Telephone:+49 (0) 721 - 56 06 0 **Telefax:** +49 (0) 721 - 56 06 149 **e-mail:** sicherheit@carlroth.de **Website:** www.carlroth.de

Competent person responsible for the safety data Department Health, Safety and Environment sheet:

e-mail (competent person):

sicherheit@carlroth.de

1.4 Emergency telephone number

Name	Street	Postal code/city	Telephone	Website
NSW Poisons Information Centre Childrens Hospital	Hawkesbury Road	2145 West- mead, NSW	131126	

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification acc. to GHS

Section	Hazard class	Cat- egory	Hazard class and category	Hazard statement
3.10	Acute toxicity (oral)	4	Acute Tox. 4	H302
3.3	Serious eye damage/eye irritation	2	Eye Irrit. 2	H319

For full text of abbreviations: see SECTION 16

2.2 Label elements

date of compilation: 2019-10-11 Revision: 2024-03-02

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Labelling	
Signal word	Warning
Pictograms	
GHS07	
Hazard statemer	its
H302 H319	Harmful if swallowed Causes serious eye irritation
Precautionary st	atements
Precautionary st	atements - prevention
P270 P280	Do not eat, drink or smoke when using this product Wear eye protection/face protection
Precautionary st	atements - response
P305+P351+P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
P330 P337+P313	Rinse mouth If eye irritation persists: Get medical advice/attention
Precautionary st	atements - disposal
P501	Dispose of contents/container to industrial combustion plant
Other hazards	
Endocrine disrup	ting properties
Does not contain	an endocrine disruptor (ED) at a concentration of \geq 0,1%.

3.1 Substances

Name of substance	Acetophenone
Molecular formula	C ₈ H ₈ O
Molar mass	120.2 ^g / _{mol}
CAS No	98-86-2

SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

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Take off contaminated clothing.

Following inhalation

Provide fresh air. In all cases of doubt, or when symptoms persist, seek medical advice.

Following skin contact

Rinse skin with water/shower. In all cases of doubt, or when symptoms persist, seek medical advice.

Following eye contact

Irrigate copiously with clean, fresh water for at least 10 minutes, holding the eyelids apart. In case of eye irritation consult an ophthalmologist.

Following ingestion

Rinse mouth with water (only if the person is conscious). Call a doctor.

4.2 Most important symptoms and effects, both acute and delayed

Vomiting, Irritation, Malaise

4.3 Indication of any immediate medical attention and special treatment needed none

SECTION 5: Firefighting measures

5.1 Extinguishing media



Suitable extinguishing media

co-ordinate firefighting measures to the fire surroundings! water spray, alcohol resistant foam, dry extinguishing powder, BC-powder, carbon dioxide (CO₂)

Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Combustible.

Hazardous combustion products

In case of fire may be liberated: Carbon monoxide (CO), Carbon dioxide (CO₂)

5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures



For non-emergency personnel

Avoid contact with skin, eyes and clothes. Do not breathe vapour/spray.

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6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose of it.

6.3 Methods and material for containment and cleaning up

Advice on how to contain a spill

Covering of drains.

Advice on how to clean up a spill

Absorb with liquid-binding material (sand, diatomaceous earth, acid- or universal binding agents).

Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

6.4 Reference to other sections

Hazardous combustion products: see section 5. Personal protective equipment: see section 8. Incompatible materials: see section 10. Disposal considerations: see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Provision of sufficient ventilation.

Advice on general occupational hygiene

Wash hands before breaks and after work. Keep away from food, drink and animal feedingstuffs.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice:

Specific designs for storage rooms or vessels

Recommended storage temperature: 15 - 25 °C

7.3 Specific end use(s)

No information available.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

National limit values

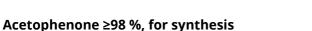
Occupational exposure limit values (Workplace Exposure Limits)

This information is not available.

Human health values

Relevant DN	Relevant DNELs and other threshold levels				
Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time	
DNEL	1.23 mg/m ³	human, inhalatory	worker (industry)	chronic - systemic effects	

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Relevant DN	Relevant DNELs and other threshold levels				
Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time	
DNEL	0.35 mg/kg bw/ day	human, dermal	worker (industry)	chronic - systemic effects	

Environmental values

Relevant PNECs and other threshold levels				
End- point	Threshold level	Organism	Environmental com- partment	Exposure time
PNEC	0.086 ^{mg} / _l	aquatic organisms	freshwater	short-term (single instance)
PNEC	0.009 ^{mg} / _l	aquatic organisms	marine water	short-term (single instance)
PNEC	34.6 ^{mg} / _l	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)
PNEC	1.13 ^{mg} / _{kg}	aquatic organisms	freshwater sediment	short-term (single instance)
PNEC	0.113 ^{mg} / _{kg}	aquatic organisms	marine sediment	short-term (single instance)
PNEC	0.175 ^{mg} / _{kg}	terrestrial organisms	soil	short-term (single instance)

8.2 Exposure controls

Individual protection measures (personal protective equipment)

Eye/face protection



Use safety goggle with side protection.

Skin protection



hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves. The times are approximate values from measurements at 22 ° C and permanent contact. Increased temperatures due to heated substances, body heat etc. and a reduction of the effective layer thickness by stretching can lead to a consider-able reduction of the breakthrough time. If in doubt, contact manufacturer. At an approx. 1.5 times larger / smaller layer thickness, the respective breakthrough time is doubled / halved. The data apply only to the pure substance. When transferred to substance mixtures, they may only be considered as a guide.

• type of material

Butyl caoutchouc (butyl rubber)

material thickness

0,7mm

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• breakthrough times of the glove material

>480 minutes (permeation: level 6)

• other protection measures

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended.

Respiratory protection



Respiratory protection necessary at: Aerosol or mist formation. Type: A (against organic gases and vapours with a boiling point of > 65 $^{\circ}$ C, colour code: Brown).

Environmental exposure controls

Keep away from drains, surface and ground water.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Physical state	liquid
Colour	colourless
Odour	mild sweet
Melting point/freezing point	20 °C (ECHA)
Boiling point or initial boiling point and boiling range	202 °C at 1,013 hPa (ECHA)
Flammability	this material is combustible, but will not ignite readily
Lower and upper explosion limit	1.4 vol% (LEL) - 5.2 vol% (UEL)
Flash point	105 °C (ECHA)
Auto-ignition temperature	535 °C at 1,013 hPa (ECHA) (auto-ignition temper- ature (liquids and gases))
Decomposition temperature	not relevant
pH (value)	not determined
Kinematic viscosity	not determined
Dynamic viscosity	1.681 mPa s at 25 °C
Solubility(ies)	
Water solubility	6.3 ^g / _l at 25 °C (ECHA)
Partition coefficient	
Partition coefficient n-octanol/water (log value):	1.63 (ECHA)
Soil organic carbon/water (log KOC)	0.973 (ECHA)

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	Vapour pressure	0.45 hPa at 25 °C
		0.45 m d dt 25 °C
	Density and/or relative density	
	Density	1.03 ^g / _{cm³} at 20 °C (ECHA)
	Relative vapour density	Information on this property is not available.
	Particle characteristics	not relevant (liquid)
	Other safety parameters	
	Oxidising properties	none
9.2	Other information	
	Information with regard to physical hazard classes:	hazard classes acc. to GHS (physical hazards): not relevant
	Other safety characteristics:	
	Surface tension	39.04 ^{mN} / _m (25 °C) (ECHA)

10.1 Reactivity

In case of warming: Vapours may form explosive mixtures with air.

If heated

Vapours may form explosive mixtures with air.

10.2 Chemical stability

The material is stable under normal ambient and anticipated storage and handling conditions of temperature and pressure.

10.3 Possibility of hazardous reactions

Violent reaction with: strong oxidiser, Strong alkali, Reducing agent

10.4 Conditions to avoid

Keep away from heat.

10.5 Incompatible materials

There is no additional information.

10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

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SECTION 11: Toxicological information

11.1 Information on toxicological effects

Classification acc. to GHS

Acute toxicity

Harmful if swallowed.

GHS of the United Nations, annex 4. May be harmful in contact with skin.

Acute toxicity					
Exposure route	Endpoint	Value	Species	Method	Source
oral	LD50	2,081 ^{mg} / _{kg}	rat		ECHA
dermal	LD50	3,300 ^{mg} / _{kg}	rat		ECHA

Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.

Serious eye damage/eye irritation

Causes serious eye irritation.

Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

Germ cell mutagenicity

Shall not be classified as germ cell mutagenic.

Carcinogenicity

Shall not be classified as carcinogenic.

Reproductive toxicity

Shall not be classified as a reproductive toxicant.

Specific target organ toxicity - single exposure

Shall not be classified as a specific target organ toxicant (single exposure).

Specific target organ toxicity - repeated exposure

Shall not be classified as a specific target organ toxicant (repeated exposure).

Aspiration hazard

Shall not be classified as presenting an aspiration hazard.

Symptoms related to the physical, chemical and toxicological characteristics

• If swallowed

vomiting, nausea

• If in eyes

Causes serious eye irritation

• If inhaled

cough, pain, choking, and breathing difficulties

• If on skin

irritant effects

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Other information

none

11.2 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of $\ge 0,1\%$.

SECTION 12: Ecological information

12.1 Toxicity

Harmful to aquatic life.

Aquatic toxicity (acute)						
Endpoint	Value	Species	Source	Exposure time		
LC50	162 ^{mg} / _l	fish	ECHA	96 h		
EC50	162 ^{mg} / _l	fish	ECHA	96 h		
ErC50	86.4 ^{mg} / _l	algae	ECHA	72 h		

12.2 Persistence and degradability

Theoretical Oxygen Demand: 2.53 ^{mg}/_{mg} Theoretical Carbon Dioxide: 2.93 ^{mg}/_{mg}

Biodegradation

The substance is readily biodegradable.

Process of degradability				
Process	Degradation rate	Time		
oxygen depletion	64.7 %	14 d		
DOC removal	<30 %	28 d		

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol	/water (log KOW)	1.63 (ECHA)
BCF		0.475 (ECHA)

12.4 Mobility in soil

Henry's law constant	0.766 ^{Pa m³} / _{mol} at 20 °C (ECHA)
The Organic Carbon normalised adsorption coefficient	0.973 (ECHA)

12.5 Results of PBT and vPvB assessment

Data are not available.

12.6 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of $\ge 0,1\%$.

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12.7 Other adverse effects

Data are not available.

SECTION 13: Disposal considerations

13.1 Waste treatment methods



This material and its container must be disposed of as hazardous waste. Dispose of contents/container in accordance with local/regional/national/international regulations.

Sewage disposal-relevant information

Do not empty into drains.

Waste treatment of containers/packagings

Handle contaminated packages in the same way as the substance itself. Completely emptied packages can be recycled.

13.3 Remarks

Waste shall be separated into the categories that can be handled separately by the local or national waste management facilities. Please consider the relevant national or regional provisions. Non-contaminated packages may be recycled.

SECTION 14: Transport information

- 14.1 UN number
- 14.2 UN proper shipping name
- 14.3 Transport hazard class(es)
- 14.4 Packing group
- 14.5 Environmental hazards

not subject to transport regulations

not assigned

not assigned

not assigned

non-environmentally hazardous acc. to the dangerous goods regulations

- **14.6 Special precautions for user** There is no additional information.
- 14.7 Transport in bulk according to IMO instruments

The cargo is not intended to be carried in bulk.

14.8 Information for each of the UN Model Regulations

Transport informationNational regulationsAdditional information(UN RTDG) Not subject to transport regulations. UN RTDG

International Maritime Dangerous Goods Code (IMDG) - Additional information Not subject to IMDG.

International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information Not subject to ICAO-IATA.

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SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture There is no additional information.

National regulations(Australia)

Australian Inventory of Chemical Substances(AICS)

Substance is listed.

Other information

Directive 94/33/EC on the protection of young people at work. Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

Country	Inventory	Status
AU	AIIC	substance is listed
CA	DSL	substance is listed
CN	IECSC	substance is listed
EU	ECSI	substance is listed
EU	REACH Reg.	substance is listed
JP	CSCL-ENCS	substance is listed
KR	KECI	substance is listed
MX	INSQ	substance is listed
NZ	NZIoC	substance is listed
PH	PICCS	substance is listed
TR	CICR	substance is listed
TW	TCSI	substance is listed
US	TSCA	substance is listed (ACTIVE)
VN	NCI	substance is listed

National inventories

Legend

AIIC Australian Inventory of Industrial Chemicals CICR Chemical Inventory and Control Regulation CSCL-ENCS List of Existing and New Chemical Substances (CSCL-ENCS) DSL Domestic Substances List (DSL) ECSI EC Substance Inventory (EINECS, ELINCS, NLP) IECSC Inventory of Existing Chemical Substances Produced or Imported in China INSQ National Inventory of Chemical Substances KECI Korea Existing Chemicals Inventory NCI National Chemical Inventory NCI National Chemical Inventory NCI New Zealand Inventory of Chemicals PICCS Philippine Inventory of Chemicals and Chemical Substances (PICCS) REACH Reg. REACH registered substances TCSI Taiwan Chemical Substance Inventory TSCA Toxic Substance Control Act

15.2 Chemical Safety Assessment

No Chemical Safety Assessment has been carried out for this substance.

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SECTION 16: Other information

Indication of changes (revised safety data sheet)

Section	Former entry (text/value)	Actual entry (text/value)	Safety- relev- ant
2.3	Results of PBT and vPvB assessment: According to the results of its assessment, this substance is not a PBT or a vPvB.		yes
2.3		Endocrine disrupting properties: Does not contain an endocrine disruptor (ED) at a concentration of ≥ 0,1%.	yes
15.1		National inventories: change in the listing (table)	yes

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
BCF	Bioconcentration factor
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
DGR	Dangerous Goods Regulations (see IATA/DGR)
DNEL	Derived No-Effect Level
EC50	Effective Concentration 50 %. The EC50 corresponds to the concentration of a tested substance causing 50 % changes in response (e.g. on growth) during a specified time interval
ED	Endocrine disruptor
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
ErC50	= EC50: in this method, that concentration of test substance which results in a 50 % reduction in either growth (EbC50) or growth rate (ErC50) relative to the control
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Na- tions
IATA	International Air Transport Association
IATA/DGR	Dangerous Goods Regulations (DGR) for the air transport (IATA)
ICAO	International Civil Aviation Organization
IMDG	International Maritime Dangerous Goods Code
LC50	Lethal Concentration 50%: the LC50 corresponds to the concentration of a tested substance causing 50 % lethality during a specified time interval
LD50	Lethal Dose 50 %: the LD50 corresponds to the dose of a tested substance causing 50 % lethality during a specified time interval
LEL	Lower explosion limit (LEL)
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
UEL	Upper explosion limit (UEL)
UN RTDG	UN Recommendations on the Transport of Dangerous Good

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Abbr.	Descriptions of used abbreviations
vPvB	Very Persistent and very Bioaccumulative

Key literature references and sources for data

Safe Work Australia's Code of Practice for Labelling of Workplace Hazardous Chemicals (under WHS Regulations).

UN Recommendations on the Transport of Dangerous Good. International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

List of relevant phrases (code and full text as stated in section 2 and 3)

Code	Text
H302	Harmful if swallowed.
H319	Causes serious eye irritation.

Disclaimer

This information is based upon the present state of our knowledge. This SDS has been compiled and is solely intended for this product.