

according to Regulation (EC) No. 1907/2006

Revision Date 05.02.2015

Version 5.2

# SECTION 1. Identification of the substance/mixture and of the company/undertaking

1.1 Product identifier

Catalogue No. 820161

Product name 4,4'-Bis(diethylamino)-benzophenone for synthesis

REACH Registration Number A registration number is not available for this substance as the

substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a

later registration deadline.

CAS-No. 90-93-7

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

Identified uses Chemical for synthesis

For additional information on uses please refer to the Merck Chemicals

portal (www.merckgroup.com).

1.3 Details of the supplier of the safety data sheet

Company Merck KGaA \* 64271 Darmstadt \* Germany \* Phone: +49 6151 72-0

Responsible Department LS-QHC \* e-mail: prodsafe@merckgroup.com

1.4 Emergency telephone

number

Please contact the regional company representation in your country.

# **SECTION 2. Hazards identification**

# 2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

Eye irritation, Category 2, H319

Chronic aquatic toxicity, Category 2, H411

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

Classification (67/548/EEC or 1999/45/EC)

Xi Irritant R36 N Dangerous for the environment R51/53

For the full text of the R-phrases mentioned in this Section, see Section 16.

### 2.2 Label elements

# Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms





Signal word Warning

according to Regulation (EC) No. 1907/2006

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Product name 4,4'-Bis(diethylamino)-benzophenone for synthesis

### Hazard statements

H319 Causes serious eye irritation.

H411 Toxic to aquatic life with long lasting effects.

### Precautionary statements

Prevention

P273 Avoid release to the environment.

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.

#### Reduced labelling (≤125 ml)

Hazard pictograms





Signal word Warning

*CAS-No.* 90-93-7

### 2.3 Other hazards

None known.

# SECTION 3. Composition/information on ingredients

# 3.1 Substance

Formula  $4-[C_2H_5)_2N]C_6H_4-COC_6H_4-4-[N(C_2H_5)_2]$   $C_{21}H_{28}N_2O$  (Hill)

EC-No. 202-025-4 Molar mass 324,46 g/mol

# Hazardous components (REGULATION (EC) No 1272/2008)

Chemical Name (Concentration)

CAS-No. Registration number Classification 4,4'-bis(diethylamino)benzophenone (<= 100 %)

90-93-7 \*)

Eye irritation, Category 2, H319

Chronic aquatic toxicity, Category 2, H411

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

# Hazardous components (1999/45/EC)

Chemical Name (Concentration)
CAS-No. Classification

4,4'-bis(diethylamino)benzophenone (<= 100 %)

90-93-7 Xi, Irritant; R36

N, Dangerous for the environment; R51/53

For the full text of the R-phrases mentioned in this Section, see Section 16.

<sup>\*)</sup> A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

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### 3.2 Mixture

Not applicable

#### **SECTION 4. First aid measures**

### 4.1 Description of first aid measures

After inhalation: fresh air.

After skin contact: wash off with plenty of water. Remove contaminated clothing.

After eye contact: rinse out with plenty of water. Call in ophthalmologist.

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

# 4.2 Most important symptoms and effects, both acute and delayed

Irritation and corrosion

### 4.3 Indication of any immediate medical attention and special treatment needed

No information available.

# **SECTION 5. Firefighting measures**

## 5.1 Extinguishing media

Suitable extinguishing media

Water, Carbon dioxide (CO2), Foam, Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

# 5.2 Special hazards arising from the substance or mixture

Combustible material

Vapours are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or vapours possible in the event of fire.

Fire may cause evolution of:

nitrogen oxides

# 5.3 Advice for firefighters

Special protective equipment for firefighters

In the event of fire, wear self-contained breathing apparatus.

Further information

Prevent fire extinguishing water from contaminating surface water or the ground water system.

Suppress (knock down) gases/vapours/mists with a water spray jet.

### SECTION 6. Accidental release measures

# 6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid substance contact. Avoid inhalation of dusts. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders: Protective equipment see section 8.

### 6.2 Environmental precautions

Do not empty into drains.

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# 6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills.

Observe possible material restrictions (see sections 7 and 10).

Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

### 6.4 Reference to other sections

Indications about waste treatment see section 13.

# SECTION 7. Handling and storage

# 7.1 Precautions for safe handling

Advice on safe handling

Observe label precautions.

Hygiene measures

Change contaminated clothing. Wash hands after working with substance.

### 7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Protected from light. Tightly closed. Dry.

Recommended storage temperature see product label.

# 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

# 8.2 Exposure controls

# Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

See section 7.1.

# Individual protection measures

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

Eye/face protection

Safety glasses

Hand protection

full contact:

Glove material: Nitrile rubber Glove thickness: 0,11 mm Preak through time: > 480 min

splash contact:

Glove material: Nitrile rubber Glove thickness: 0,11 mm Break through time: > 480 min

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Product name 4,4'-Bis(diethylamino)-benzophenone for synthesis

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 741 Dermatril® L (full contact), KCL 741 Dermatril® L (splash contact).

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

This recommendation applies only to the product stated in the safety data sheet<(>,<)> supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Other protective equipment protective clothing

Respiratory protection

required when dusts are generated.

Recommended Filter type: Filter P 1 (acc. to DIN 3181) for solid particles of inert substances. The entrepeneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

# Environmental exposure controls

Do not empty into drains.

# SECTION 9. Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

Form powder, finecrystalline

Colour yellow

Odour odourless

Odour Threshold No information available.

pH 4 - 6

at 50 g/l 20 °C

Melting point 90 - 95 °C

Boiling point No information available.

Flash point 151 °C

Method: DIN 51758

Evaporation rate No information available.

Flammability (solid, gas) No information available.

Lower explosion limit No information available.

Upper explosion limit No information available.

Vapour pressure No information available.

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Relative vapour density No information available.

Density No information available.

Relative density No information available.

Water solubility at 20 °C

slightly soluble

log Pow: 5,47

Partition coefficient: n-

octanol/water (calculated)

(Lit.) A remarkable bioaccumulation potential is expected (log

Po/w > 3).

Auto-ignition temperature No information available.

Decomposition temperature > 360 °C

Viscosity, dynamic No information available.

Explosive properties No information available.

Oxidizing properties No information available.

9.2 Other data

Bulk density 400 kg/m<sup>3</sup>

# SECTION 10. Stability and reactivity

# 10.1 Reactivity

Forms explosive mixtures with air on intense heating.

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

### 10.2 Chemical stability

Decomposes on exposure to light.

# 10.3 Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents

nitrosing agents, nitrous acid, nitrites

Nitrosamine

### 10.4 Conditions to avoid

Strong heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

# 10.5 Incompatible materials

no information available

# 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 oral toxicity

LD50 Rat: 5.000 mg/kg (External MSDS)

Acute inhalation toxicity

This information is not available.

Acute dermal toxicity

This information is not available.

Skin irritation

Rabbit

Result: No irritation (External MSDS)

Eve irritation

Rabbit

Result: Eye irritation (External MSDS)

Causes serious eye irritation.

Sensitisation

This information is not available.

Germ cell mutagenicity

This information is not available.

Carcinogenicity

This information is not available.

Reproductive toxicity

This information is not available.

Teratogenicity

This information is not available.

Specific target organ toxicity - single exposure

This information is not available.

Specific target organ toxicity - repeated exposure

This information is not available.

Aspiration hazard

This information is not available.

### 11.2 Further information

Under given conditions, contact with nitrites or nitric acid can lead to the formation of nitrosamines, which have shown themselves to be carcinogenic in animal experiments.

Further data:

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

# **SECTION 12. Ecological information**

# 12.1 Toxicity

Toxicity to fish

LC50 Leuciscus idus (Golden orfe): 1,0 - 2,2 mg/l; 96 h (External MSDS)

Toxicity to daphnia and other aquatic invertebrates

EC50 Daphnia (water flea): 1,6 mg/l; 48 h (External MSDS)

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Catalogue No. 820161

Product name 4,4'-Bis(diethylamino)-benzophenone for synthesis

Toxicity to algae

IC50 algae: 51 mg/l; 72 h (External MSDS)

## 12.2 Persistence and degradability

No information available.

### 12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 5,47 (calculated)

(Lit.) A remarkable bioaccumulation potential is expected (log Po/w >3).

### 12.4 Mobility in soil

No information available.

### 12.5 Results of PBT and vPvB assessment

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

#### 12.6 Other adverse effects

Additional ecological information

Discharge into the environment must be avoided.

# **SECTION 13. Disposal considerations**

Waste treatment methods

See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

# **SECTION 14. Transport information**

Land transport (ADR/RID)

**14.1 UN number** UN 3077

**14.2 Proper shipping name** ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID,

N.O.S. (4,4-BIS(DIETHYLAMINO)-BENZOPHENONE)

14.3 Class914.4 Packing groupIII14.5 Environmentally hazardousyes14.6 Special precautions foryes

usei

Tunnel restriction code E

Packages smaller than or equal to 5 kg / L, not dangerous goods of Class 9

# Inland waterway transport (ADN)

Not relevant

Air transport (IATA)

**14.1 UN number** UN 3077

**14.2 Proper shipping name** ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID,

N.O.S. (4,4-BIS(DIETHYLAMINO)-BENZOPHENONE)

14.3 Class914.4 Packing groupIII14.5 Environmentally hazardousyes

according to Regulation (EC) No. 1907/2006

Catalogue No. 820161

Product name 4,4'-Bis(diethylamino)-benzophenone for synthesis

14.6 Special precautions for

no

user

Packages smaller than or equal to 5 kg / L, not dangerous goods of Class 9

Sea transport (IMDG)

**14.1 UN number** UN 3077

**14.2 Proper shipping name** ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID,

N.O.S. (4,4-BIS(DIETHYLAMINO)-BENZOPHENONE)

14.3 Class914.4 Packing groupIII14.5 Environmentally hazardousyes14.6 Special precautions foryes

user

EmS F-A S-F

Packages smaller than or equal to 5 kg / L , not dangerous goods of Class 9

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not relevant

# **SECTION 15. Regulatory information**

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

EU regulations

Major Accident Hazard 96/82/EC

Legislation Dangerous for the environment

9b

Quantity 1: 200 t Quantity 2: 500 t

Occupational restrictions Take note of Dir 94/33/EC on the protection of young people at

work.

Regulation (EC) No 1005/2009 on substances that not regulated

deplete the ozone layer

Regulation (EC) No 850/2004 of the European not regulated

Parliament and of the Council of 29 April 2004 on persistent organic pollutants and amending

Directive 79/117/EEC

Regulation (EC) No 689/2008 concerning the export not regulated

and import of dangerous chemicals

Substances of very high concern (SVHC)

This product does not contain substances

of very high concern according to

Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of  $\geq$  0.1 % (w/w).

National legislation

Storage class 10 - 13

# 15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out.

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Catalogue No. 820161

Product name 4,4'-Bis(diethylamino)-benzophenone for synthesis

#### **SECTION 16. Other information**

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

H319 Causes serious eye irritation.

H411 Toxic to aquatic life with long lasting effects.

# Full text of R-phrases referred to under sections 2 and 3

R36 Irritating to eyes.

R51/53 Toxic to aquatic organisms, may cause long-term adverse effects

in the aquatic environment.

### Training advice

Provide adequate information, instruction and training for operators.

## Labelling

Hazard pictograms





Signal word
Warning

### Hazard statements

H319 Causes serious eye irritation.

H411 Toxic to aquatic life with long lasting effects.

# Precautionary statements

Prevention

P273 Avoid release to the environment.

Response

S-phrase(s)

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact

lenses, if present and easy to do. Continue rinsing.

# Labelling (67/548/EEC or 1999/45/EC)

Symbol(s) Xi Irritant N Dange

*R-phrase(s)* 36-51/53 Irritating to eyes. Toxic to aquatic organisms, may cause

long-term adverse effects in the aquatic environment.

long-term adverse effects in the aquatic environment.

Avoid release to the environment. Refer to special

instructions/ Safety data sheets.

Dangerous for the environment

EC-No. 202-025-4

Reduced labelling (≤125 ml)

Symbol(s) Irritant

Xi Dangerous for the environment

### Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at www.wikipedia.org.

according to Regulation (EC) No. 1907/2006

Catalogue No. 820161

Product name 4,4'-Bis(diethylamino)-benzophenone for synthesis

# Regional representation

This information is given on the authorised Safety Data Sheet for your country.

The information contained herein is based on the present state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.