

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 21.07.2018

Version 4.8

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

### 1.1 Product identifier

Catalogue No. 807044

Product name Phenylacetylene 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. 536-74-3

### 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](http://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](mailto:prodsafe@merckgroup.com)

1.4 Emergency telephone number Please contact the regional company representation in your country.

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## SECTION 2. Hazards identification

### 2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

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Flammable liquid, Category 3, H226

Skin irritation, Category 2, H315

Eye irritation, Category 2, H319

Aspiration hazard, Category 1, H304

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

## 2.2 Label elements

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

#### *Hazard pictograms*



#### *Signal word*

Danger

#### *Hazard statements*

H226 Flammable liquid and vapour.

H304 May be fatal if swallowed and enters airways.

H315 Causes skin irritation.

H319 Causes serious eye irritation.

#### *Precautionary statements*

##### Prevention

P210 Keep away from heat.

##### Response

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

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

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

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## Reduced labelling (≤125 ml)

### Hazard pictograms



### Signal word

Danger

### Hazard statements

H304 May be fatal if swallowed and enters airways.

### Precautionary statements

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

CAS-No. 536-74-3

## 2.3 Other hazards

None known.

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## SECTION 3. Composition/information on ingredients

### 3.1 Substance

Formula	C <sub>8</sub> H <sub>6</sub> (Hill)
EC-No.	208-645-1
Molar mass	102,13 g/mol

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

#### Chemical name (Concentration)

CAS-No.	Registration number	Classification
phenylacetylene (>= 50 % - <= 100 % )		

536-74-3 \*)

Flammable liquid, Category 3, H226

Skin irritation, Category 2, H315

Eye irritation, Category 2, H319

Aspiration hazard, Category 1, H304

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1,4-Dioxane (< 1 % )

*Substance does not meet the criteria for PBT or vPvB according to Regulation (EC) No 1907/2006, Annex XIII.*

123-91-1	01-2119462837-26-XXXX	Flammable liquid, Category 2, H225 Eye irritation, Category 2, H319 Carcinogenicity, Category 2, H351 Specific target organ toxicity - single exposure, Category 3, H335
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\*) 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.

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

## 3.2 Mixture

Not applicable

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## SECTION 4. First aid measures

### 4.1 Description of first aid measures

After inhalation: fresh air.

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/shower.

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

After swallowing: caution if victim vomits. Risk of aspiration! Keep airways free. Call a physician immediately. Pulmonary failure possible after aspiration of vomit.

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

irritant effects

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

No information available.

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## SECTION 5. Firefighting measures

### 5.1 Extinguishing media

*Suitable extinguishing media*

Foam, Carbon dioxide (CO<sub>2</sub>), 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.

Forms explosive mixtures with air at elevated temperatures.

Vapours are heavier than air and may spread along floors.

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

### 5.3 Advice for firefighters

*Special protective equipment for firefighters*

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

*Further information*

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system. Suppress (knock down) gases/vapours/mists with a water spray jet.

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## SECTION 6. Accidental release measures

### 6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapours, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. 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 let product enter drains. Risk of explosion.

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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 carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

## 6.4 Reference to other sections

Indications about waste treatment see section 13.

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## SECTION 7. Handling and storage

### 7.1 Precautions for safe handling

#### *Advice on safe handling*

Observe label precautions.

#### *Advice on protection against fire and explosion*

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

#### *Hygiene measures*

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

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

#### *Storage conditions*

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

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.

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## SECTION 8. Exposure controls/personal protection

### 8.1 Control parameters

#### **Derived No Effect Level (DNEL)**

##### *1,4-Dioxane (123-91-1)*

Worker DNEL, longterm	Local effects	inhalation	144 mg/m <sup>3</sup>
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Worker DNEL, longterm	Systemic effects	inhalation	73 mg/m <sup>3</sup>
Worker DNEL, longterm	Systemic effects	dermal	21 mg/kg Body weight

## Predicted No Effect Concentration (PNEC)

### *1,4-Dioxane (123-91-1)*

PNEC Fresh water	10 mg/l
PNEC Fresh water sediment	37 mg/kg
PNEC Marine water	0,67 mg/l
PNEC Aquatic intermittent release	10 mg/l
PNEC Sewage treatment plant	2700 mg/l
PNEC Soil	0,153 mg/kg

## 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:	butyl-rubber
Glove thickness:	0,7 mm

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Break through time:	> 480 min
splash contact:	
Glove material:	Nitrile rubber
Glove thickness:	0,40 mm
Break through time:	> 30 min

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 898 Butoject® (full contact), KCL 730 Camatril® -Velours (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](http://www.kcl.de)).

#### *Other protective equipment*

Flame retardant antistatic protective clothing.

#### *Respiratory protection*

required when vapours/aerosols are generated.

Recommended Filter type: filter ABEK

The entrepreneur 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 let product enter drains.

Risk of explosion.

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## **SECTION 9. Physical and chemical properties**

### **9.1 Information on basic physical and chemical properties**

Form	liquid
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Colour	yellow
Odour	odourless
Odour Threshold	Not applicable
pH	No information available.
Melting point	-44,8 °C
Boiling point/boiling range	142 - 144 °C at 1.013 hPa
Flash point	27 °C
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	2,7 hPa at 25 °C
Relative vapour density	3,5
Density	0,93 g/cm <sup>3</sup> at 20 °C
Relative density	No information available.

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Water solubility	0,46 g/l at 25 °C
Partition coefficient: n-octanol/water	log Pow: 2,53 (experimental) Bioaccumulation is not expected. (Lit.)
Auto-ignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	0,88 mPa.s at 25 °C
Explosive properties	Not classified as explosive.
Oxidizing properties	none

## 9.2 Other data

none

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## SECTION 10. Stability and reactivity

### 10.1 Reactivity

Vapour/air-mixtures are explosive at intense warming.

### 10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

### 10.3 Possibility of hazardous reactions

Violent reactions possible with:

Oxidizing agents, halogens, Alkali metals, perchloric acid, acids

### 10.4 Conditions to avoid

Heating.

### 10.5 Incompatible materials

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The Safety Data Sheets for catalogue items are available at [www.merckgroup.com](http://www.merckgroup.com)

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no information available

## 10.6 Hazardous decomposition products

no information available

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## SECTION 11. Toxicological information

### 11.1 Information on toxicological effects

#### *Acute oral toxicity*

LDLO Rat: 9.300 mg/kg

Symptoms: Risk of aspiration upon vomiting., Aspiration may cause pulmonary oedema and pneumonitis.

Irritation of mucous membranes

#### *Acute inhalation toxicity*

Symptoms: Possible damages:, mucosal irritations

#### *Acute dermal toxicity*

This information is not available.

#### *Skin irritation*

Causes skin irritation.

#### *Eye irritation*

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.

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## *Specific target organ toxicity - single exposure*

This information is not available.

## *Specific target organ toxicity - repeated exposure*

This information is not available.

## *Aspiration hazard*

Aspiration hazard, Aspiration may cause pulmonary oedema and pneumonitis.

### **11.2 Further information**

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

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## **SECTION 12. Ecological information**

### **12.1 Toxicity**

No information available.

### **12.2 Persistence and degradability**

No information available.

### **12.3 Bioaccumulative potential**

*Partition coefficient: n-octanol/water*

log Pow: 2,53

(experimental)

Bioaccumulation is not expected. (Lit.)

### **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.

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## SECTION 13. Disposal considerations

### *Waste treatment methods*

See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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## SECTION 14. Transport information

### Land transport (ADR/RID)

14.1 UN number	UN 1993
14.2 Proper shipping name	FLAMMABLE LIQUID, N.O.S. (PHENYLACETYLENE)
14.3 Class	3
14.4 Packing group	III
14.5 Environmentally hazardous	--
14.6 Special precautions for user	yes
Tunnel restriction code	D/E

### Inland waterway transport (ADN)

Not relevant

### Air transport (IATA)

14.1 UN number	UN 1993
14.2 Proper shipping name	FLAMMABLE LIQUID, N.O.S. (PHENYLACETYLENE)
14.3 Class	3
14.4 Packing group	III
14.5 Environmentally hazardous	--
14.6 Special precautions for user	no

### Sea transport (IMDG)

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14.1 UN number	UN 1993
14.2 Proper shipping name	FLAMMABLE LIQUID, N.O.S. (PHENYLACETYLENE)
14.3 Class	3
14.4 Packing group	III
14.5 Environmentally hazardous	--
14.6 Special precautions for user	yes
EmS	F-E S-E

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

Not relevant

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## SECTION 15. Regulatory information

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

#### *EU regulations*

Major Accident Hazard	SEVESO III
Legislation	FLAMMABLE LIQUIDS
	P5c
	Quantity 1: 5.000 t
	Quantity 2: 50.000 t

Occupational restrictions	Take note of Dir 94/33/EC on the protection of young people at work.
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Regulation (EC) No 1005/2009 on substances that deplete the ozone layer	not regulated
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Regulation (EC) No 850/2004 of the European Parliament and of the Council of 29 April 2004 on persistent organic pollutants and amending Directive 79/117/EEC	not regulated
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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 3

## 15.2 Chemical safety assessment

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

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## SECTION 16. Other information

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

H225	Highly flammable liquid and vapour.
H226	Flammable liquid and vapour.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
H351	Suspected of causing cancer.

### Training advice

Provide adequate information, instruction and training for operators.

### 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](http://www.wikipedia.org).

### Regional representation

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

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*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.*