

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 26.09.2017

Version 5.3

SECTION 1. Identification of the substance/mixture and of the company/undertaking**1.1 Product identifier**

Catalogue No. 820555

Product name Hexyl acetate 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. 142-92-7

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)**

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Flammable liquid, Category 3, H226

Chronic aquatic toxicity, Category 2, H411

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

Warning

Hazard statements

H226 Flammable liquid and vapour.

H411 Toxic to aquatic life with long lasting effects.

Precautionary statements

Prevention

P210 Keep away from heat.

P273 Avoid release to the environment.

Reduced labelling (≤ 125 ml)

Hazard pictograms



Signal word

Warning

Index-No. 607-462-00-8

2.3 Other hazards

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None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

Formula $C_8H_{16}O_2$ (Hill)
Index-No. 607-462-00-8
EC-No. 205-572-7
EC-No. 421-230-1
Molar mass 144,21 g/mol

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

Chemical name (Concentration)

CAS-No. Registration number Classification

hexyl acetate ($\leq 100\%$)

142-92-7 *)

Flammable liquid, Category 3, H226

Chronic aquatic toxicity, Category 2, H411

*) 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

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.

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

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

4.2 Most important symptoms and effects, both acute and delayed

irritant effects, Nausea, Vomiting, Stomach/intestinal disorders

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

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.

Vapours are heavier than air and may spread along floors.

Forms explosive mixtures with air at elevated temperatures.

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

5.3 Advice for firefighters

Special protective equipment for firefighters

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

Further information

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6. Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

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Advice for non-emergency personnel: Do not breathe vapours, aerosols. 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.

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 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.

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

Change contaminated clothing. Wash hands after working with substance.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed.

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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.

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

splash contact:

Glove material:	butyl-rubber
Glove thickness:	0,7 mm
Break through time:	> 60 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® (splash contact).

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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

Flame retardant antistatic protective clothing.

Respiratory protection

required when vapours/aerosols are generated.

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

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.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Form	liquid
Colour	colourless
Odour	aromatic
Odour Threshold	No information available.
pH	No information available.
Melting point	-80 °C

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Boiling point/boiling range	171,5 °C at 1.013 hPa
Flash point	56 °C Method: c.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	5 hPa at 20 °C
Relative vapour density	No information available.
Density	0,87 g/cm ³ at 20 °C
Relative density	No information available.
Water solubility	0,4 g/l at 20 °C
Partition coefficient: n-octanol/water	log Pow: 2,83 (calculated) Bioaccumulation is not expected. (Lit.)
Auto-ignition temperature	No information available.
Decomposition temperature	No information available.

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Viscosity, dynamic	No information available.
Explosive properties	Not classified as explosive.
Oxidizing properties	none

9.2 Other data

none

SECTION 10. Stability and reactivity

10.1 Reactivity

Explosible with air in a vaporous/gaseous state when heated.
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:
Strong oxidizing agents

10.4 Conditions to avoid

Heating.

10.5 Incompatible materials

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

LD50 Rat: 36.100 mg/kg

(RTECS)

Symptoms: Nausea, Stomach/intestinal disorders, Vomiting, Risk of aspiration upon vomiting.,
Aspiration may cause pulmonary oedema and pneumonitis.

Acute inhalation toxicity

This information is not available.

Acute dermal toxicity

LD50 Rabbit: > 5.000 mg/kg

(RTECS)

Skin irritation

Rabbit

Result: slight irritation

(RTECS)

Eye irritation

Rabbit

Result: slight irritation

(RTECS)

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.

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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

However, when the product is handled appropriately, hazardous effects are unlikely to occur.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

12.1 Toxicity

Toxicity to fish

LC50 Pimephales promelas (fathead minnow): 4,4 mg/l; 96 h

(External MSDS)

12.2 Persistence and degradability

Biodegradability

66 %; 28 d

(External MSDS)

Readily biodegradable

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 2,83

(calculated)

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.

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12.6 Other adverse effects

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 3272
14.2 Proper shipping name	ESTERS, N.O.S. (HEXYL ACETATE)
14.3 Class	3
14.4 Packing group	III
14.5 Environmentally hazardous	yes
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 3272
14.2 Proper shipping name	ESTERS, N.O.S. (HEXYL ACETATE)
14.3 Class	3
14.4 Packing group	III
14.5 Environmentally hazardous	yes
14.6 Special precautions for user	no

Sea transport (IMDG)

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14.1 UN number UN 3272
14.2 Proper shipping name ESTERS, N.O.S. (HEXYL ACETATE)
14.3 Class 3
14.4 Packing group III
14.5 Environmentally hazardous yes
14.6 Special precautions for user yes
EmS F-E S-D
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 SEVESO III
Legislation FLAMMABLE LIQUIDS
P5c
Quantity 1: 5.000 t
Quantity 2: 50.000 t

SEVESO III
ENVIRONMENTAL HAZARDS
E2
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 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

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 ≥ 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.

SECTION 16. Other information

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

H226 Flammable liquid and vapour.
H411 Toxic to aquatic life with long lasting effects.

Training advice

Provide adequate information, instruction and training for operators.

Labelling

Hazard pictograms



Signal word

Warning

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Precautionary statements

Prevention

P210 Keep away from heat.

P273 Avoid release to 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.

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.