

Safety Data Sheet

Essigsäureanhydrid-d6

According to Regulation (EC) No. 1907/2006 (REACH)

Classification acc. to 29 CFR 1910.1200

Version number: GHS 2.1
Replaces version of: 2022-03-23 (GHS 1)

Revision: 2023-02-02

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

1.1 Product identifier

Identification of the substance	Essigsäureanhydrid-d6
CAS number	16649-49-3
Alternative name(s)	(² H ₃)acetyl (² H ₃)acetate

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

Relevant identified uses	laboratory and analytical use laboratory chemical
HS code	2845.90.

1.3 Details of the supplier of the safety data sheet

Zeochem AG Joweid 5, CH-8630 Rüti Switzerland	Telephone: +41 44 922 93 93 e-Mail: info@zeochem.com / info@zeochem.ch Website: https://www.zeochem.com
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1.4 Emergency telephone number

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification acc. to GHS

Section	Hazard class	Category	Hazard class and category	Hazard statement
2.6	flammable liquid	3	Flam. Liq. 3	H226
3.10	acute toxicity (oral)	4	Acute Tox. 4	H302
3.11	acute toxicity (inhal.)	4	Acute Tox. 4	H332
3.2	skin corrosion/irritation	1B	Skin Corr. 1B	H314
3.3	serious eye damage/eye irritation	1	Eye Dam. 1	H318

For full text of abbreviations: see SECTION 16.

The most important adverse physicochemical, human health and environmental effects

Skin corrosion produces an irreversible damage to the skin; namely, visible necrosis through the epidermis and into the dermis. The product is combustible and can be ignited by potential ignition sources.

2.2 Label elements

Labelling

- Signal word danger

Safety Data Sheet

Essigsäureanhydrid-d6

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Revision: 2023-02-02

2.2.1.2 Pictograms

GHS02, GHS05, GHS07	  
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Hazard statements	
H226	flammable liquid and vapour
H302+H332	harmful if swallowed or if inhaled
H314	causes severe skin burns and eye damage

Precautionary statements	
P210	keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking
P260	do not breathe dust/fume/gas/mist/vapours/spray
P280	wear protective gloves/protective clothing/eye protection/face protection/hearing protection
P303+P361+P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower
P305+P351+P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
P310	immediately call a POISON CENTER/doctor
P370+P378	in case of fire: Use sand, carbon dioxide or powder extinguisher to extinguish
P403+P235	store in a well-ventilated place. Keep cool

2.3 Other hazards

Results of PBT and vPvB assessment

According to the results of its assessment, this substance is not a PBT or a vPvB.

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance	Essigsäureanhydrid-d6
Identifiers	
CAS No	16649-49-3
EC No	240-697-0
Purity	>99 %

Safety Data Sheet

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Specific Conc. Limits	M-Factors	ATE	Exposure route
Skin Corr. 1B; H314: $C \geq 25\%$ Skin Irrit. 2; H315: $5\% \leq C < 25\%$ Eye Dam. 1; H318: $5\% \leq C < 25\%$ Eye Irrit. 2; H319: $1\% \leq C < 5\%$	-	630 mg/kg 11 mg/l/4h	oral inhalation: vapour

Molecular formula

C4D6O3

Molar mass

108 g/mol

SECTION 4: First aid measures

4.1 Description of first aid measures

General notes

Do not leave affected person unattended. Remove victim out of the danger area. Keep affected person warm, still and covered. Take off immediately all contaminated clothing. In all cases of doubt, or when symptoms persist, seek medical advice. In case of unconsciousness place person in the recovery position. Never give anything by mouth.

Following inhalation

If breathing is irregular or stopped, immediately seek medical assistance and start first aid actions. In case of respiratory tract irritation, consult a physician. Provide fresh air.

Following skin contact

Wash with plenty of soap and water.

Following eye contact

Remove contact lenses, if present and easy to do. Continue rinsing. Irrigate copiously with clean, fresh water for at least 10 minutes, holding the eyelids apart.

Following ingestion

Rinse mouth with water (only if the person is conscious). Do NOT induce vomiting.

4.2 Most important symptoms and effects, both acute and delayed

Symptoms and effects are not known to date.

4.3 Indication of any immediate medical attention and special treatment needed

none

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water spray, Alcohol resistant foam, BC-powder, Carbon dioxide (CO2)

Unsuitable extinguishing media

Water jet

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Revision: 2023-02-02

5.2 Special hazards arising from the substance or mixture

In case of insufficient ventilation and/or in use, may form flammable/explosive vapour-air mixture. Solvent vapours are heavier than air and may spread along floors. Places which are not ventilated, e.g. unventilated below ground level areas such as trenches, conduits and shafts, are particularly prone to the presence of flammable substances or mixtures.

Hazardous combustion products

Carbon monoxide (CO), Carbon dioxide (CO₂)

5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. Co-ordinate firefighting measures to the fire surroundings. Do not allow firefighting water to enter drains or water courses. Collect contaminated firefighting water separately. Fight fire with normal precautions from a reasonable distance.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

For non-emergency personnel

Remove persons to safety.

For emergency responders

Wear breathing apparatus if exposed to vapours/dust/spray/gases.

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

Wipe up with absorbent material (e.g. cloth, fleece). Collect spillage: sawdust, kieselgur (diatomite), sand, universal binder

Appropriate containment techniques

Use of adsorbent materials.

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.

Safety Data Sheet

Essigsäureanhydrid-d6

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Version number: GHS 2.1
Replaces version of: 2022-03-23 (GHS 1)

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SECTION 7: Handling and storage

7.1 Precautions for safe handling

Recommendations

Store in a dry place.

- Measures to prevent fire as well as aerosol and dust generation

Use local and general ventilation. Avoidance of ignition sources. Keep away from sources of ignition - No smoking. Take precautionary measures against static discharge. Use only in well-ventilated areas. Due to danger of explosion, prevent leakage of vapours into cellars, flues and ditches. Ground/bond container and receiving equipment. Use explosion-proof electrical/ventilating/lighting/equipment. Use only non-sparking tools.

- Specific notes/details

Places which are not ventilated, e.g. unventilated below ground level areas such as trenches, conduits and shafts, are particularly prone to the presence of flammable substances or mixtures. Vapours are heavier than air, spread along floors and form explosive mixtures with air. Vapours may form explosive mixtures with air.

Advice on general occupational hygiene

Wash hands after use. Do not eat, drink and smoke in work areas. Remove contaminated clothing and protective equipment before entering eating areas. Never keep food or drink in the vicinity of chemicals. Never place chemicals in containers that are normally used for food or drink. Keep away from food, drink and animal feedingstuffs.

7.2 Conditions for safe storage, including any incompatibilities

Managing of associated risks

- Explosive atmospheres

Keep container tightly closed and in a well-ventilated place. Use local and general ventilation. Keep cool. Protect from sunlight.

- Flammability hazards

Keep away from sources of ignition - No smoking. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Take precautionary measures against static discharge. Protect from sunlight.

- Ventilation requirements

Keep any substance that emits harmful vapours or gases in a place that allows these to be permanently extracted. Use local and general ventilation. Ground/bond container and receiving equipment.

- Packaging compatibilities

Only packagings which are approved (e.g. acc. to ADR) may be used.

7.3 Specific end use(s)

See section 16 for a general overview.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Safety Data Sheet

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Classification acc. to 29 CFR 1910.1200

Version number: GHS 2.1

Replaces version of: 2022-03-23 (GHS 1)

Revision: 2023-02-02

Occupational exposure limit values (Workplace Exposure Limits)

Country	Name of agent	CAS No	Identifier	TWA [ppm]	TWA [mg/m ³]	STEL [ppm]	STEL [mg/m ³]	Ceiling-C [ppm]	Ceiling-C [mg/m ³]	Notation	Source
GB	acetic anhydride	108-24-7	WEL	0.5	2.5	2	10				EH40/2005

Notation

Ceiling-C
STEL ceiling value is a limit value above which exposure should not occur
short-term exposure limit: a limit value above which exposure should not occur and which is related to a 15-minute period (unless otherwise specified)

TWA time-weighted average (long-term exposure limit): measured or calculated in relation to a reference period of 8 hours
time-weighted average (unless otherwise specified)

8.2 Exposure controls

Appropriate engineering controls

General ventilation.

Individual protection measures (personal protective equipment)

Eye/face protection

Wear eye/face protection.

Skin protection

- Hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. Check leak-tightness/impermeability prior to use. In the case of wanting to use the gloves again, clean them before taking off and air them well. 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.

- Type of material

Nitrile

IIR: isobutene-isoprene (butyl) rubber

- Breakthrough times of the glove material

>30 minutes (permeation: level 2)

- Other protection measures

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended. Wash hands thoroughly after handling.

Respiratory protection

In case of inadequate ventilation wear respiratory protection.

Environmental exposure controls

Use appropriate container to avoid environmental contamination. Keep away from drains, surface and ground water.

Safety Data Sheet

Essigsäureanhydrid-d6

According to Regulation (EC) No. 1907/2006 (REACH)

Classification acc. to 29 CFR 1910.1200

Version number: GHS 2.1
Replaces version of: 2022-03-23 (GHS 1)

Revision: 2023-02-02

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Physical state	liquid
Colour	not determined
Odour	characteristic
Melting point/freezing point	-73 °C
Boiling point or initial boiling point and boiling range	140 °C at 101 kPa
Flammability	flammable liquid in accordance with GHS criteria
Lower and upper explosion limit	2.7 vol% - 10.3 vol%
Flash point	49 °C at 101 hPa (closed cup)
Auto-ignition temperature	316 °C at 101 hPa (ECHA)
Decomposition temperature	not relevant
pH (value)	not determined
Kinematic viscosity	not determined

Solubility(ies)

Water solubility	120 g/l at 20 °C
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Partition coefficient

Partition coefficient n-octanol/water (log value)	-0.577 (pH value: 7, 25 °C) (ECHA)
Soil organic carbon/water (log KOC)	0.146 (ECHA)

Vapour pressure	10 kPa at 75.1 °C
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Safety Data Sheet

Essigsäureanhydrid-d6

According to Regulation (EC) No. 1907/2006 (REACH)

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Version number: GHS 2.1
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Revision: 2023-02-02

Density and/or relative density

Density	1.15 g/cm ³ at 20 °C
Relative vapour density	information on this property is not available

Particle characteristics	not relevant (liquid)
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9.2 Other information

Information with regard to physical hazard classes	there is no additional information
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Other safety characteristics

Surface tension	31.9 mN/m (25 °C) (ECHA)
Refractive index	1.39 (20 °C) ((lit.))

SECTION 10: Stability and reactivity

10.1 Reactivity

Concerning incompatibility: see below "Conditions to avoid" and "Incompatible materials". It's a reactive substance. The mixture contains reactive substance(s). Risk of ignition.

If heated:

Risk of ignition

10.2 Chemical stability

See below "Conditions to avoid".

10.3 Possibility of hazardous reactions

No known hazardous reactions.

10.4 Conditions to avoid

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

Hints to prevent fire or explosion

Use explosion-proof electrical/ventilating/lighting/equipment. Use only non-sparking tools. Take precautionary measures against static discharge.

10.5 Incompatible materials

Oxidisers

10.6 Hazardous decomposition products

Reasonably anticipated hazardous decomposition products produced as a result of use, storage, spill and heating are not known. Hazardous combustion products: see section 5.

Safety Data Sheet

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Version number: GHS 2.1

Replaces version of: 2022-03-23 (GHS 1)

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SECTION 11: Toxicological information

11.1 Information on toxicological effects

Classification acc. to GHS

Acute toxicity

Harmful if swallowed. Harmful if inhaled.

- Acute toxicity estimate (ATE)

Oral	630 mg/kg
Inhalation: vapour	11 mg/l/4h

Skin corrosion/irritation

Causes severe skin burns and eye damage.

Serious eye damage/eye irritation

Causes serious eye damage.

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.

11.2 Information on other hazards

There is no additional information.

SECTION 12: Ecological information

12.1 Toxicity

Shall not be classified as hazardous to the aquatic environment.

Safety Data Sheet

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Revision: 2023-02-02

12.2 Persistence and degradability

Biodegradation

The substance is readily biodegradable.

12.3 Bioaccumulative potential

Data are not available.

n-octanol/water (log KOW)	-0.577 (pH value: 7, 25 °C) (ECHA)
BCF	3.16 (ECHA)

12.4 Mobility in soil

Henry's law constant	0.817 Pa m ³ /mol at 25 °C
The Organic Carbon normalised adsorption coefficient	0.146 (ECHA)

12.5 Results of PBT and vPvB assessment

Data are not available.

12.6 Endocrine disrupting properties

Not listed.

12.7 Other adverse effects

Data are not available.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Waste treatment-relevant information

Solvent reclamation/regeneration.

Sewage disposal-relevant information

Do not empty into drains. Avoid release to the environment. Refer to special instructions/safety data sheets.

Waste treatment of containers/packagegings

It is a dangerous waste; only packagegings which are approved (e.g. acc. to ADR) may be used. Completely emptied packagegings can be recycled. Handle contaminated packagegings in the same way as the substance itself.

Remarks

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

Safety Data Sheet

Essigsäureanhydrid-d6

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Version number: GHS 2.1
Replaces version of: 2022-03-23 (GHS 1)

Revision: 2023-02-02

SECTION 14: Transport information

14.1 UN number or ID number

ADR/RID	UN 1715
IMDG-Code	UN 1715
ICAO-TI	UN 1715

14.2 UN proper shipping name

ADR/RID	ACETIC ANHYDRIDE
IMDG-Code	ACETIC ANHYDRIDE
ICAO-TI	Acetic anhydride

14.3 Transport hazard class(es)

ADR/RID	8 (3)
IMDG-Code	8 (3)
ICAO-TI	8 (3)

14.4 Packing group

ADR/RID	II
IMDG-Code	II
ICAO-TI	II

14.5 Environmental hazards

non-environmentally hazardous acc. to the dangerous goods regulations

14.6 Special precautions for user

Provisions for dangerous goods (ADR) should be complied within the premises.

14.7 Maritime transport in bulk according to IMO instruments

The cargo is not intended to be carried in bulk.

Information for each of the UN Model Regulations

Agreement concerning the International Carriage of Dangerous Goods by Road (ADR) - Additional information

Classification code	CF1
Danger label(s)	8+3



Excepted quantities (EQ)	E2
Limited quantities (LQ)	1 L
Transport category (TC)	2

Safety Data Sheet

Essigsäureanhydrid-d6

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Version number: GHS 2.1

Replaces version of: 2022-03-23 (GHS 1)

Revision: 2023-02-02

Tunnel restriction code (TRC) D/E

Hazard identification No 83

Emergency Action Code 3W

Regulations concerning the International Carriage of Dangerous Goods by Rail (RID) - Additional information

Classification code CF1

Danger label(s) 8+3



Excepted quantities (EQ) E2

Limited quantities (LQ) 1 L

Transport category (TC) 2

Hazard identification No 83

International Maritime Dangerous Goods Code (IMDG) - Additional information

Marine pollutant -

Danger label(s) 8+3



Excepted quantities (EQ) E2

Limited quantities (LQ) 1 L

EmS F-E, S-C

Stowage category A

Segregation group 1 - Acids

International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information

Danger label(s) 8+3



Excepted quantities (EQ) E2

Limited quantities (LQ) 0,5 L

Safety Data Sheet

Essigsäureanhydrid-d6

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Version number: GHS 2.1

Replaces version of: 2022-03-23 (GHS 1)

Revision: 2023-02-02

SECTION 15: Regulatory information

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

Relevant provisions of the European Union (EU)

Directive on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS)

not listed

Regulation concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

Water Framework Directive (WFD)

not listed

Regulation on persistent organic pollutants (POP)

Not listed.

National regulations (GB)

List of substances subject to authorisation (GB REACH, Annex 14) / SVHC - candidate list

not listed

Restrictions according to GB REACH, Annex 17

Dangerous substances with restrictions (GB REACH, Annex 17)			
Name of substance	Name acc. to inventory	CAS No	No
Essigsäureanhydrid-d6	this product meets the criteria for classification in accordance with Regulation No 1272/2008/EC		3
Essigsäureanhydrid-d6	flammable / pyrophoric		40

National inventories

Country	Inventory	Status
EU	REACH Reg.	substance is listed
US	TSCA	substance is listed

Legend

REACH Reg. REACH registered substances
TSCA Toxic Substance Control Act

15.2 Chemical Safety Assessment

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

Safety Data Sheet

Essigsäureanhydrid-d6

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Version number: GHS 2.1
Replaces version of: 2022-03-23 (GHS 1)

Revision: 2023-02-02

SECTION 16: Other information

Key literature references and sources for data

Agreement concerning the International Carriage of Dangerous Goods by Road (ADR). Regulations concerning the International Carriage of Dangerous Goods by Rail (RID). 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
H226	Flammable liquid and vapour.
H302	Harmful if swallowed.
H314	Causes severe skin burns and eye damage.
H318	Causes serious eye damage.
H332	Harmful if inhaled.

Disclaimer

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