



Safety data sheet

according to 1907/2006/EC, Article 31

Printing date 30.12.2022

version: 1

Revision: 30.12.2022

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

1.1 Product identifier:

Trade name: **Dodeca 2E,4E,8Z,10E,Z-tetraenoic acid isobutylamide (in acetonitrile)**

Article number: 89187

CAS Number: 866602-52-0 (Dodeca 2E,4E,8Z,10E,Z-tetraenoic acid isobutylamide)

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

No further relevant information available.

Application of the substance / the preparation: Reference substance

1.3 Details of the supplier of the safety data sheet:

Manufacturer/Supplier:

PhytoLab GmbH & Co. KG

Dutendorfer Str. 5-7

D-91487 Vestenbergsgreuth

Tel.: Germany/9163/88-327

Fax: Germany/9163/88-456

Mail: ref-substances@phytolab.de

Further information obtainable from: PLV_MSDS@phytolab.com

1.4 Emergency telephone number: Germany/9163/88-500

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture:

Classification according to Regulation (EC) No 1272/2008:



GHS02 flame

Flam. Liq. 2 H225 Highly flammable liquid and vapour.



GHS07

Acute Tox. 4 H302 Harmful if swallowed.

Acute Tox. 4 H312 Harmful in contact with skin.

Acute Tox. 4 H332 Harmful if inhaled.

Eye Irrit. 2 H319 Causes serious eye irritation.

2.2 Label elements:

Labelling according to Regulation (EC) No 1272/2008:

The product is classified and labelled according to the CLP regulation.

Hazard pictograms:



GHS02 GHS07

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Signal word: Danger

Hazard-determining components of labelling:

acetonitrile

Hazard statements:

H225 Highly flammable liquid and vapour.

H302+H312+H332 Harmful if swallowed, in contact with skin or if inhaled.

H319 Causes serious eye irritation.

Precautionary statements

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

P241 Use explosion-proof [electrical/ventilating/lighting] equipment.

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.

P403+P235 Store in a well-ventilated place. Keep cool.

P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

2.3 Other hazards:

Restricted to professional users. The toxicological properties of this compound have not been fully evaluated.

Results of PBT and vPvB assessment:

PBT: Not applicable.

vPvB: Not applicable.

SECTION 3: Composition/information on ingredients

3.2 Mixtures

Description:

Mixture: consisting of the following components.

Mixture of substances listed below with nonhazardous additions.

Significant substances:

Dodeca 2E,4E,8Z,10E,Z-tetraenoic acid isobutylamide (10 mg in 1 ml acetonitrile)

Synonyms: 2,4,8,10-Dodecatetraenamide, N-(2-methylpropyl)-, (2E,4E,8Z,10E)-, mixt. with (2E,4E,8Z,10Z)-N-(2-methylpropyl)-2,4,8,10-dodecatetraenamide (9CI)

Molecular formula: C₁₆H₂₅NO

Dangerous components:

CAS: 75-05-8	acetonitrile	≥40%
EINECS: 200-835-2	⚠ Flam. Liq. 2, H225; ⚠ Acute Tox. 4, H302; Acute	
Index number: 608-001-00-3	Tox. 4, H312; Acute Tox. 4, H332; Eye Irrit. 2, H319	
Reg.nr.: 01-2119471307-38-XXXX		

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Additional information: For the wording of the listed hazard phrases refer to section 16.

SECTION 4: First aid measures

4.1 Description of first aid measures:

General information:

Induce vomiting only with medical help.

Immediately remove any clothing soiled by the product.

After inhalation: Supply fresh air and to be sure call for a doctor.

After skin contact:

Immediately rinse with water.

If skin irritation continues, consult a doctor.

After eye contact:

Rinse opened eye for several minutes under running water. If symptoms persist, consult a doctor.

After swallowing:

Rinse out mouth and then drink plenty of water.

If symptoms persist consult doctor.

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

No further relevant information available.

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

No further relevant information available.

SECTION 5: Firefighting measures

5.1 Extinguishing media:

Suitable extinguishing agents:

CO₂, powder or water spray. Fight larger fires with water spray or alcohol resistant foam.

Use fire extinguishing methods suitable to surrounding conditions.

For safety reasons unsuitable extinguishing agents: Water with full jet

5.2 Special hazards arising from the substance or mixture:

No further relevant information available.

5.3 Advice for firefighters:

Protective equipment:

Wear self-contained respiratory protective device.

Wear fully protective suit.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures:

Ensure adequate ventilation

Use respiratory protective device against the effects of fumes/dust/aerosol.

Wear protective equipment. Keep unprotected persons away.

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6.2 Environmental precautions: Do not allow to enter sewers/ surface or ground water.

6.3 Methods and material for containment and cleaning up:

Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).

Dispose contaminated material as waste according to item 13.

Ensure adequate ventilation.

6.4 Reference to other sections:

See Section 7 for information on safe handling.

See Section 8 for information on personal protection equipment.

See Section 13 for disposal information.

SECTION 7: Handling and storage

7.1 Precautions for safe handling:

Handling corresponding to laboratory safety guidelines.

Keep receptacles tightly sealed.

Ensure good ventilation/exhaustion at the workplace.

Prevent formation of aerosols.

Information about fire - and explosion protection:

Keep ignition sources away - Do not smoke.

Protect against electrostatic charges.

7.2 Conditions for safe storage, including any incompatibilities:

Storage:

Requirements to be met by storerooms and receptacles: Store in a cool location.

Information about storage in one common storage facility: Store away from foodstuffs.

Further information about storage conditions:

Store in the dark.

Keep container tightly sealed.

Store in cool, dry conditions in well sealed receptacles.

Recommended storage temperature: < -15 °C

Storage class: 3

7.3 Specific end use(s): No further relevant information available.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters:

Ingredients with limit values that require monitoring at the workplace:

75-05-8 acetonitrile

IOELV Long-term value: 70 mg/m³, 40 ppm

Skin

Additional information: The lists valid during the making were used as basis.

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8.2 Exposure controls:

Appropriate engineering controls: No further data; see item 7.

Individual protection measures, such as personal protective equipment:

General protective and hygienic measures:

Keep away from foodstuffs, beverages and feed.

Immediately remove all soiled and contaminated clothing

Wash hands before breaks and at the end of work.

Avoid contact with the eyes and skin.

Respiratory protection:

Suitable respiratory protective device recommended.

In case of brief exposure or low pollution use respiratory filter device. In case of intensive or longer exposure use self-contained respiratory protective device.

Hand protection:

The glove material has to be impermeable and resistant to the product/ the substance/ the preparation.

Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation

Material of gloves:



Butyl rubber, BR

The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.

Penetration time of glove material:

The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.

Eye/face protection:



Tightly sealed goggles

Body protection: Protective work clothing

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties:

General Information:

Physical state:

Fluid

Colour:

According to Certificate of Analysis

Odour:

No data available.

Odour threshold:

Not determined.

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Molecular Weight

Melting point/freezing point: -46 °C

Boiling point or initial boiling point and boiling range:

81 °C

Flammability: Highly flammable.

Dust explosion class:

Lower and upper explosion limit:

Lower: 4.4 Vol %

Upper: 16 Vol %

Flash point: 12.8 °C (closed cup)

(Minimum) Ignition temperature: 525 °C

Decomposition temperature: Not determined.

Powder volume resistivity:

pH: Not determined.

Dissociation constant:

Viscosity:

Kinematic viscosity: Not determined.

Solubility in other solvents:

Dynamic: Not determined.

Solubility:

water: No data available.

Partition coefficient n-octanol/water (log value): Not determined.

Vapour pressure at 20 °C: 97 hPa

Density and/or relative density:

Density at 20 °C: 0.7822 g/cm³

Relative density: Not determined.

Vapour density: Not determined.

9.2 Other information:

Appearance:

Form: Liquid

Important information on protection of health and environment, and on safety.

Auto-ignition temperature: Product is not selfigniting.

Explosive properties: Product is not explosive. However, formation of explosive air/vapour mixtures are possible.

Molecular weight: 41.05 g/mol

Oxidising properties: Not determined.

Evaporation rate: Not determined.

Information with regard to physical hazard classes:

Explosives: Void

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Flammable gases	Void
Aerosols	Void
Oxidising gases	Void
Gases under pressure	Void
Flammable liquids	Highly flammable liquid and vapour.
Flammable solids	Void
Self-reactive substances and mixtures	Void
Pyrophoric liquids	Void
Pyrophoric solids	Void
Self-heating substances and mixtures	Void
Substances and mixtures, which emit flammable gases in contact with water	Void
Oxidising liquids	Void
Oxidising solids	Void
Organic peroxides	Void
Corrosive to metals	Void
Desensitised explosives	Void

SECTION 10: Stability and reactivity

- 10.1 Reactivity: No further relevant information available.
- 10.2 Chemical stability:
Thermal decomposition / conditions to be avoided:
Stable under constant-temperature (see 7.)
- 10.3 Possibility of hazardous reactions: No data available.
- 10.4 Conditions to avoid: No further relevant information available.
- 10.5 Incompatible materials: Strong oxidising agents.
- 10.6 Hazardous decomposition products: no data available

SECTION 11: Toxicological information

- 11.1 Information on hazard classes as defined in Regulation (EC) No 1272/2008
Acute toxicity: Harmful if swallowed, in contact with skin or if inhaled.
LD/LC50 values relevant for classification:
Quantitative data on the toxicity of the product are not available.

ATE (Acute Toxicity Estimates)

- Oral LD50 505 mg/kg
Dermal LD50 1,263 mg/kg (rabbit)
Inhalative LC50/4 h 11.1 mg/l

75-05-8 acetonitrile

- Oral LD50 2,730 mg/kg (rat)

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Dermal LD50 1,250 mg/kg (rabbit)

Inhalative LC50/4 h 11 mg/l (ATE)

Skin corrosion/irritation: Based on available data, the classification criteria are not met.

Serious eye damage/irritation: Causes serious eye irritation.

Respiratory or skin sensitisation:

Based on available data, the classification criteria are not met.

Germ cell mutagenicity: Based on available data, the classification criteria are not met.

Carcinogenicity: Based on available data, the classification criteria are not met.

Reproductive toxicity: Based on available data, the classification criteria are not met.

STOT-single exposure: Based on available data, the classification criteria are not met.

STOT-repeated exposure: Based on available data, the classification criteria are not met.

Aspiration hazard: Based on available data, the classification criteria are not met.

Additional toxicological information:

The product should be handled with the care usual when dealing with chemicals.

11.2 Information on other hazards

Endocrine disrupting properties:

None of the ingredients is listed.

SECTION 12: Ecological information

12.1 Toxicity:

Aquatic toxicity:

Quantitative data concerning the ecological properties of the product are not available.

12.2 Persistence and degradability: No further relevant information available.

12.3 Bioaccumulative potential: No further relevant information available.

12.4 Mobility in soil: No further relevant information available.

12.5 Results of PBT and vPvB assessment:

PBT: Not applicable.

vPvB: Not applicable.

12.6 Endocrine disrupting properties:

The product does not contain substances with endocrine disrupting properties.

12.7 Other adverse effects:

Remark: Do not release into sewage, water or soil.

Additional ecological information:

General notes:

Water hazard class 2 (German Regulation) (Self-assessment): hazardous for water

Do not allow product to reach ground water, water course or sewage system.

Danger to drinking water if even small quantities leak into the ground.

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SECTION 13: Disposal considerations

13.1 Waste treatment methods:

Recommendation:

Dispose product and packaging in accordance with regional environmental laws.

Must not be disposed together with household garbage. Do not allow product to reach sewage system.

Uncleaned packaging:

Recommendation: Disposal must be made according to official regulations.

SECTION 14: Transport information

14.1 UN number or ID number:

ADR, IMDG, IATA

UN1648

14.2 UN proper shipping name:

ADR

IMDG, IATA

UN1648 ACETONITRILE

ACETONITRILE

14.3 Transport hazard class(es):

ADR, IMDG, IATA



Class

3 Flammable liquids.

Label

3

14.4 Packing group:

ADR, IMDG, IATA

II

14.5 Environmental hazards:

Marine pollutant:

No

14.6 Special precautions for user:

Warning: Flammable liquids.

Hazard identification number (Kemler code):

33

EMS Number:

F-E, S-D

Stowage Category

B

Stowage Code

SW2 Clear of living quarters.

14.7 Maritime transport in bulk according to

IMO instruments:

Not applicable.

Transport/Additional information:

ADR

Limited quantities (LQ)

1L

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Excepted quantities (EQ)

Code: E2

Maximum net quantity per inner packaging: 30 ml

Maximum net quantity per outer packaging: 500 ml

Transport category

2

Tunnel restriction code

D/E

IMDG

Limited quantities (LQ)

1L

Excepted quantities (EQ)

Code: E2

Maximum net quantity per inner packaging: 30 ml

Maximum net quantity per outer packaging: 500 ml

UN "Model Regulation":

UN 1648 ACETONITRILE, 3, II

SECTION 15: Regulatory information

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

Directive 2012/18/EU:

Named dangerous substances - ANNEX I: None of the ingredients is listed.

Seveso category P5c FLAMMABLE LIQUIDS

Qualifying quantity (tonnes) for the application of lower-tier requirements 5,000 t

Qualifying quantity (tonnes) for the application of upper-tier requirements 50,000 t

REGULATION (EC) No 1907/2006 ANNEX XVII Conditions of restriction: 3

DIRECTIVE 2011/65/EU on the restriction of the use of certain hazardous substances in electrical and electronic equipment – Annex II:

None of the ingredients is listed.

REGULATION (EU) 2019/1148

Annex I - RESTRICTED EXPLOSIVES PRECURSORS (Upper limit value for the purpose of licensing under Article 5(3)):

None of the ingredients is listed.

Annex II - REPORTABLE EXPLOSIVES PRECURSORS:

None of the ingredients is listed.

National regulations:

Information about limitation of use:

When using chemicals, legal regulations have to be regarded (chemical law, maternity protection, protection of minors).

Waterhazard class: Water hazard class 2 (Self-assessment): hazardous for water.

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15.2 Chemical safety assessment: A Chemical Safety Assessment has not been carried out.

SECTION 16: Other information

This information is based on our present knowledge. However, this shall not constitute a guarantee for any specific product features and shall not establish a legally valid contractual relationship.

Relevant phrases:

H225 Highly flammable liquid and vapour.

H302 Harmful if swallowed.

H312 Harmful in contact with skin.

H319 Causes serious eye irritation.

H332 Harmful if inhaled.

Classification according to Regulation (EC) No 1272/2008

Flammable liquids

On basis of test data

Acute toxicity - oral

Acute toxicity - dermal

Acute toxicity - inhalation

The classification of the mixture is generally based on the calculation method using substance data according to Regulation (EC) No 1272/2008.

Serious eye damage/eye irritation

Abbreviations and acronyms:

RID: Règlement international concernant le transport des marchandises dangereuses par chemin de fer (Regulations Concerning the International Transport of Dangerous Goods by Rail)

IATA-DGR: Dangerous Goods Regulations by the "International Air Transport Association" (IATA)

ICAO: International Civil Aviation Organisation

ICAO-TI: Technical Instructions by the "International Civil Aviation Organisation" (ICAO)

ADR: Accord relatif au transport international des marchandises dangereuses par route (European Agreement Concerning the International Carriage of Dangerous Goods by Road)

IMDG: International Maritime Code for Dangerous Goods

IATA: International Air Transport Association

GHS: Globally Harmonised System of Classification and Labelling of Chemicals

EINECS: European Inventory of Existing Commercial Chemical Substances

ELINCS: European List of Notified Chemical Substances

CAS: Chemical Abstracts Service (division of the American Chemical Society)

LC50: Lethal concentration, 50 percent

LD50: Lethal dose, 50 percent

PBT: Persistent, Bioaccumulative and Toxic

vPvB: very Persistent and very Bioaccumulative

Flam. Liq. 2: Flammable liquids – Category 2

Acute Tox. 4: Acute toxicity – Category 4

Eye Irrit. 2: Serious eye damage/eye irritation – Category 2