

According to Regulation (EC) No 1907/2006

According to Regulation (EC) No 2020/878

3,4-Dimethoxyphenethylamine

Version number: 1
Issued: 2024-04-17



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

1.1. Product identifier

Trade name

3,4-Dimethoxyphenethylamine

CAS number

120-20-7

EC number

204-376-9

Synonyms

Homoveratrylamine

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

Relevant identified uses

Research and development. Laboratory Chemicals. Manufacture of substances.

Not suitable for use in

Not suitable for human consumption or veterinary purposes.

1.3. Details of the supplier of the safety data sheet

Supplier

Molekula Group

Address

Molekula Ltd, Lingfield Way, Darlington,
DL1 4XX Darlington
United Kingdom

Telephone

+44 (0) 3302 000 333

Email

info@molekula.com

Web site

www.molekula.com

Contact person

Kevin Banks

Email

+44 (0) 7769276927

1.4. Emergency telephone number

Poison center/Additional emergency number

0344 892 0111 - National Poisons Information Service (Newcastle Centre)

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SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008

Classification

Serious eye damage, hazard category 1

Skin irritation, hazard category 2

Skin sensitisation, hazard category 1

Acute toxicity, oral, hazard category 4

Specific Target Organ Toxicity — Single exposure, hazard category 3

Hazard statements

H302, H315, H317, H318, H335

2.2. Label elements

Labelling according to Regulation (EC) No 1272/2008

Hazard pictograms



Signal word

Danger

Hazard statements

H302 Harmful if swallowed.

H315 Causes skin irritation.

H317 May cause an allergic skin reaction.

H318 Causes serious eye damage.

H335 May cause respiratory irritation.

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Precautionary statements

P261 Avoid breathing dust/fumes/gas/mist/vapours/spray.
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P271 Use only outdoors or in a well-ventilated area.
P272 Contaminated work clothing should not be allowed out of the workplace.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P301 + P312 IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell.
P302 + P352 IF ON SKIN: Wash with plenty of water/.
P304 + P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P332 + P313 If skin irritation occurs: Get medical advice/attention.
P405 Store locked up.
P403 + P233 Store in a well-ventilated place. Keep container tightly closed.
P501 Dispose of contents/container to local regulations.
P362 + P364 Take off contaminated clothing and wash it before reuse.
P333 + P313 If skin irritation or rash occurs: Get medical advice/attention.

2.3. Other hazards

No data available

SECTION 3: Composition/information on ingredients

3.2. Mixtures

| Chemical name | CAS No. EC No. REACH No. Index No. | Concentration | Classification | H-phrases M factor acute M factor chronic | Note |
|-----------------------------|---------------------------------------------|---------------|-------------------------------------------------------------------------------------|-------------------------------------------------|------|
| 3,4-Dimethoxyphenethylamine | 120-20-7 204-376-9 - - | 100% | Acute Tox. 4 - oral, Skin Irrit. 2, Skin Sens. 1, Eye Dam. 1, STOT SE 3 | H302, H315, H317, H318, H335 - - | - |

Molecular weight

181.23

Substance additional information

For the complete text of H- / EUH-statements mentioned in this section, see section 16.

SECTION 4: First aid measures

4.1. Description of first aid measures

IF exposed or concerned: Get medical advice/attention. First aiders/ medical personnel need to protect themselves. Show this Safety Data Sheet (SDS) to medical personnel.

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Inhalation

IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/doctor. If breathing stops, provide artificial respiration. For breathing difficulties oxygen may be necessary.

Skin contact

IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water [or shower]. Immediately call a POISON CENTER/doctor.

Eye contact

Remove contact lenses if present. Rinse eyes with water. Continue to rinse for at least 15 minutes and seek medical attention.

Ingestion

IF SWALLOWED: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only if the persons are fully conscious and awake). Administer activated charcoal (20 - 40g in a 10% slurry) and consult a doctor as quickly as possible. Do not attempt to neutralise.

Information for doctors

No data available.

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

The severity of the symptoms described will vary dependant of the concentration and the length of exposure. Causes burns by all exposure routes.

See section 11 for more detailed information on health effects and symptoms.

Inhalation

Single exposure may cause the following adverse effects: Causes severe burns. Difficulty in breathing. Unconsciousness, possibly death.

Skin contact

Single exposure may cause the following adverse effects: Causes severe burns. Blistering may occur. May be absorbed in the body and cause dizziness, nausea and vomiting. Unconsciousness, death.

Eye contact

Single exposure may cause the following adverse effects: Causes serious eye damage. Unconsciousness, possibly death.

Ingestion

Single exposure may cause the following adverse effects: Severe abdominal pain. May cause severe internal injury. Unconsciousness, possibly death.

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

Treat symptomatically. Immediately call a POISON CENTER/doctor.

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SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

In case of fire: Use foam, carbon dioxide, dry powder or water fog to extinguish.

Unsuitable extinguishing media

No specific fire fighting procedure given.

5.2. Special hazards arising from the substance or mixture

Specific hazards: Corrosive. Combustible.

Thermal decomposition or combustion may liberate carbon oxides and other toxic gases or vapours.

Carbon monoxide (CO). Carbon dioxide (CO₂).

Nitrous gases (NO_x).

Vapours are heavier than air and may spread near ground to sources of ignition.

Forms explosive mixtures with air on intense heating.

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

5.3. Advice for firefighters

Special protective equipment for fire-fighters

Evacuate area. Avoid breathing gas, fume, vapours or spray. Prevent skin contact by maintaining a safe distance and by wearing suitable protective equipment/ clothing. Cool containers exposed to heat with water spray and remove container, if no risk is involved.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

Do not breathe vapour/spray. Avoid contact with skin and eyes. For personal protection, see section 8.

In case of fire: Evacuate area. Fight fire remotely due to the risk of explosion.

6.2. Environmental precautions

Avoid discharge into drains, water courses or onto the ground.

6.3. Methods and material for containment and cleaning up

Collect with absorbent, non-combustible material into suitable containers.

6.4. Reference to other sections

For personal protection, see section 8. For waste disposal, see section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Preventive handling precautions

For precautions see section 2.2. Work under hood. Take action to prevent static discharges. Wear protective clothing, gloves, eye and face protection. Avoid contact with skin and eyes. Avoid ingestion and inhalation.

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General hygiene

Observe good chemical hygiene practices. Keep away from food, drink and animal feeding stuffs. Wash contaminated skin thoroughly after handling. Do not eat, drink or smoke when using this product. Remove contaminated clothing and launder thoroughly before re-use.

7.2. Conditions for safe storage, including any incompatibilities

Store in a dry place. Store in a closed container.

Recommended storage temperature: 2 to 8°C (35.6 to 46.4°F)

Hygroscopic. Store under inert gas. Air sensitive.

7.3. Specific end use(s)

No specific usage precautions noted.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

No data available

8.2. Exposure controls

Personal Protective Equipment Symbols



Eye / face protection

Wear eye protection.

Hand protection

Wear protective gloves. Recommended gloves: Butyl rubber.

Glove Thickness: 0.7mm

Breakthrough time: 8 hours

Always inspect gloves before use. If signs of wear and tear are noticed then the gloves should be replaced.

No specific hygiene procedures noted, but good personal hygiene practices are always advisable, especially when working with chemicals. Wash contaminated skin thoroughly after handling.

Other skin protection

Wash skin thoroughly after handling.

Respiratory protection

Provide adequate ventilation. If ventilation is insufficient, suitable respiratory protection must be provided.

Environmental exposure controls

Avoid discharge into drains.

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SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state

Liquid

Colour

Light yellow

Odour

Amine.

Melting point / freezing point

12 °C

Boiling point or initial boiling point and boiling range

188 °C

Flammability

0.1 - 0.7

Lower and upper explosion limit

No data available

Flash point

125 °C

Auto-ignition temperature

No data available

Decomposition temperature

290.1 °C

pH

No data available

Kinematic viscosity

No data available

Solubility

No data available

Partition coefficient n-octanol/water

0.77

Vapour pressure

0.000348

Density and/or relative density

1.09 g/cm³

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Relative vapour density

No data available

Explosive properties

Not classified as explosive.

Particle characteristics

No data available

9.2. Other information

No data available

SECTION 10: Stability and reactivity

10.1. Reactivity

Forms explosive mixtures with air on intense heating.

15 (approx) Kelvin below the flash point is to be rated as critical.

10.2. Chemical stability

Stable under the prescribed storage conditions.

10.3. Possibility of hazardous reactions

Exothermic reaction with:

Strong oxidising agents.

acid halides

Acid anhydrides.

Caution! In contact with nitrites, nitrates, nitrous acid possible liberation of nitrosamines!

10.4. Conditions to avoid

Air sensitive.

Hygroscopic. Heating.

10.5. Incompatible materials

Strong oxidising agents. Strong acids. Strong bases Acid chlorides Acid anhydrides.

10.6. Hazardous decomposition products

See section 5.

SECTION 11: Toxicological information

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Acute toxicity

| Product / Sub- stance name CAS / EC no. | Dose descriptor | Value / Dose | Exposure route | Duration of exposure | Test animals |
|-----------------------------------------------|-----------------|--------------|----------------|----------------------|--------------|
| 3,4-Dimethoxyphen- | LD50 | 720 mg/kg | Oral | - | Rat |

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| Product / Sub- stance name CAS / EC no. | Dose descriptor | Value / Dose | Exposure route | Duration of exposure | Test animals |
|-----------------------------------------------------|-----------------|--------------|----------------|----------------------|--------------|
| ethylamine 120-20-7 / 204-376-9 | | | | | |
| 3,4-Dimethoxyphenethylamine 120-20-7 / 204-376-9 | LC50 | >5.5 mg/l | Inhalation. | 4 hours | Rat |
| 3,4-Dimethoxyphenethylamine 120-20-7 / 204-376-9 | LD50 | 2800 mg/kg | Dermal | - | Rat |

Skin corrosion/irritation

| Product / Substance name CAS / EC no. | Result | Species |
|-----------------------------------------------------|--------------------|---------|
| 3,4-Dimethoxyphenethylamine 120-20-7 / 204-376-9 | Irritating to skin | Rabbit |

Serious eye damage/irritation

| Product / Substance name CAS / EC no. | Result | Species |
|-----------------------------------------------------|---------------------------------|---------|
| 3,4-Dimethoxyphenethylamine 120-20-7 / 204-376-9 | Irreversible effects on the eye | Rabbit |

Respiratory or skin sensitisation

| Product / Substance name CAS / EC no. | Result | Species | Method / Guideline |
|-----------------------------------------------------|--------------------------|---------|------------------------|
| 3,4-Dimethoxyphenethylamine 120-20-7 / 204-376-9 | May cause sensitisation. | Mouse | Local Lymph Node Assay |

Aspiration hazard

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

11.2. Information on other hazards

No data available

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SECTION 12: Ecological information

12.1. Toxicity

Acute fish toxicity

| Product / Substance name CAS / EC no. | Measurement type | Value / Result | Duration of exposure | Species |
|-----------------------------------------------------|------------------|----------------|----------------------|------------------------------|
| 3,4-Dimethoxyphenethylamine 120-20-7 / 204-376-9 | LC50 | 46 - 100 mg/l | 96 hours | Leuciscus idus (Golden orfe) |

12.2. Persistence and degradability

No data available

12.3. Bioaccumulative potential

No data available

12.4. Mobility in soil

No data available

12.5. Results of PBT and vPvB assessment

No data available

12.6. Endocrine disrupting properties

This product does not contain any known or suspected endocrine disruptors.

12.7. Other adverse effects

No data available

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Disposal considerations

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

SECTION 14: Transport information

14.1. UN number

Not applicable

14.2. UN proper shipping name

Not applicable

14.3. Transport hazard class(es)

Not applicable

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14.4. Packing group

Not applicable

14.5. Environmental hazards

Not applicable

14.6. Special precautions for user

Not applicable

14.7. Maritime transport in bulk according to IMO instruments

Not applicable

SECTION 15: Regulatory information

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

EU regulations

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

This material safety data sheet complies with the requirements of Regulation (EU) 2020/878.

National regulations

No data available

15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

SECTION 16: Other information

Phrase meaning

Eye Dam. 1 - Serious eye damage, hazard category 1

Skin Irrit. 2 - Skin irritation, hazard category 2

Skin Sens. 1 - Skin sensitisation, hazard category 1

Acute Tox. 4 - oral - Acute toxicity, oral, hazard category 4

STOT SE 3 - Specific Target Organ Toxicity — Single exposure, hazard category 3

H302 Harmful if swallowed.

H315 Causes skin irritation.

H317 May cause an allergic skin reaction.

H318 Causes serious eye damage.

H335 May cause respiratory irritation.