SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

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

1.1 Product identifier

<table>
<thead>
<tr>
<th>Catalogue No.</th>
<th>801452</th>
</tr>
</thead>
<tbody>
<tr>
<td>Product name</td>
<td>Anisole for synthesis</td>
</tr>
<tr>
<td>REACH Registration Number</td>
<td>01-2119968918-13-XXXX</td>
</tr>
<tr>
<td>CAS-No.</td>
<td>100-66-3</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Identified uses</th>
<th>Chemical for synthesis</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>In compliance with the conditions described in the annex to this safety data sheet.</td>
</tr>
</tbody>
</table>

1.3 Details of the supplier of the safety data sheet

<table>
<thead>
<tr>
<th>Company</th>
<th>Merck KGaA * 64271 Darmstadt * Germany * Phone:+49 6151 72-0</th>
</tr>
</thead>
<tbody>
<tr>
<td>Responsible Department</td>
<td>EQ-RS * e-mail: <a href="mailto:prodsafe@merckgroup.com">prodsafe@merckgroup.com</a></td>
</tr>
</tbody>
</table>

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)

Flammable liquid, Category 3, H226

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

Classification (67/548/EEC or 1999/45/EC)

R10

For the full text of the R-phrases 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.

Precautionary statements
Prevention
P210 Keep away from heat.
P262 Do not get in eyes, on skin, or on clothing.

Reduced labelling (≤125 ml)

Signal word
Warning

CAS-No. 100-66-3

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

<table>
<thead>
<tr>
<th>Formula</th>
<th>C₆H₅OCH₃</th>
<th>C₇H₈O (Hill)</th>
</tr>
</thead>
<tbody>
<tr>
<td>EC-No.</td>
<td>202-876-1</td>
<td></td>
</tr>
<tr>
<td>Molar mass</td>
<td>108.13 g/mol</td>
<td></td>
</tr>
</tbody>
</table>
SAFETY DATA SHEET
according to Regulation (EC) No. 1907/2006

Catalogue No. 801452
Product name Anisole for synthesis

Remarks No disclosure requirement according to Regulation (EC) No. 1907/2006

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.

After eye contact: rinse out with plenty of water.

After swallowing: make victim drink water (two glasses at most). Consult doctor if feeling unwell.

4.2 Most important symptoms and effects, both acute and delayed
irritant effects, Shortness of breath, agitation, spasms, Nausea, Vomiting, Headache, muscle twitching, narcosis

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
Foam, Carbon dioxide (CO2), 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

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
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)
See exposure scenario in the Annex to this MSDS.

SECTION 8. Exposure controls/personal protection

8.1 Control parameters

Derived No Effect Level (DNEL)

Worker DNEL, longterm Systemic effects inhalation 20 mg/m³

Predicted No Effect Concentration (PNEC)

PNEC Fresh water 0.027 mg/l
PNEC Marine water 0.0027 mg/l
PNEC Aquatic intermittent release 0.27 mg/l
PNEC Fresh water sediment 0.745 mg/kg
PNEC Marine sediment 0.0745 mg/kg
PNEC Soil 0.133 mg/kg
PNEC Sewage treatment plant 30 mg/l

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: Viton (R)
Glove thickness: 0,70 mm
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 890 Vitoject® (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).

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**: at 20 °C
  Not applicable
- **Melting point**: -37 °C
- **Boiling point/boiling range**: 154 °C
  at 1.013 hPa
- **Flash point**: 45,5 °C
  at 993 hPa
  Method: c.c.
- **Evaporation rate**: No information available.
- **Flammability (solid, gas)**: No information available.
- **Lower explosion limit**: 0,34 %(V)
- **Upper explosion limit**: 6,3 %(V)
- **Vapour pressure**: 3,2 hPa
  at 20 °C
Relative vapour density  3.7

Density  0.994 g/cm³
       at 20 °C

Relative density  No information available.

Water solubility  1.71 g/l
       at 20 °C
Method: OECD Test Guideline 105

Partition coefficient: n-octanol/water
log Pow: 2.62
OECD Test Guideline 117
Bioaccumulation is not expected.

Auto-ignition temperature  No information available.

Decomposition temperature  > 490 °C

Viscosity, dynamic  0.99 mPa.s
       at 25 °C

Explosive properties  Not classified as explosive.

Oxidizing properties  none

9.2 Other data

Ignition temperature  475 °C

Bulk density  Not applicable

SECTION 10. Stability and reactivity

10.1 Reactivity
Formation of peroxides possible.
Vapour/air-mixtures are explosive at intense warming.

10.2 Chemical stability
Sensitive to air.

10.3 Possibility of hazardous reactions
Violent reactions possible with:
Strong oxidizing agents, Strong acids, alkalines, formaldehyde

10.4 Conditions to avoid
Heating.

10.5 Incompatible materials
no information available

10.6 Hazardous decomposition products
Peroxides

SECTION 11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity
LD50 Rat: 3.700 mg/kg

(RTECS)

Acute inhalation toxicity
LC50 Rat: > 6,51 mg/l; 4 h ; vapour
OECD Test Guideline 403

Symptoms: Possible damages; slight mucosal irritations

Acute dermal toxicity
This information is not available.

Skin irritation
Rabbit
Result: slight irritation
OECD Test Guideline 404

Eye irritation
Rabbit
Result: No eye irritation
OECD Test Guideline 405
Sensitisation

Sensitisation test (Magnusson and Kligman):
Result: negative

(Maximisation Test (GPMT) Guinea pig
Result: negative
Method: OECD Test Guideline 406

Germ cell mutagenicity

Genotoxicity in vitro
Ames test
Escherichia coli/Salmonella typhimurium
Result: negative
Method: OECD Test Guideline 471

In vitro mammalian cell gene mutation test
Mouse lymphoma test
Result: negative
Method: OECD Test Guideline 476

Mutagenicity (mammal cell test): chromosome aberration.
Chinese hamster lung cells
Result: negative
Method: OECD Test Guideline 473

Carcinogenicity
This information is not available.

Reproductive toxicity
This information is not available.

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

Systemic effects:
After uptake of large quantities:
Nausea, Vomiting, agitation, spasms, Headache, muscle twitching, narcosis, cardiovascular
disorders
Possible damages:
Damage to:
Liver, Kidney, Central nervous system
Other dangerous properties can not be excluded.
Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

12.1 Toxicity

Toxicity to fish
LC50 Leuciscus idus (Golden orfe): > 1.000 mg/l; 96 h
(External MSDS)

Toxicity to daphnia and other aquatic invertebrates
static test EC50 Daphnia magna (Water flea): 27 mg/l; 48 h
Analytical monitoring: yes
OECD Test Guideline 202

Toxicity to algae
static test ErC50 Pseudokirchneriella subcapitata (algae): 47 mg/l; 72 h
Analytical monitoring: yes
OECD Test Guideline 201

Toxicity to bacteria
static test NOEC activated sludge: 300 mg/l; 3 h
OECD Test Guideline 209

12.2 Persistence and degradability

Biodegradability
ca. 68 %
OECD Test Guideline 301D
Readily biodegradable

Theoretical oxygen demand (ThOD)
2.520 mg/g

(Lit.)
12.3 Bioaccumulative potential

*Partition coefficient: n-octanol/water*

log Pow: 2.62

OECD Test Guideline 117

Bioaccumulation is not expected.

12.4 Mobility in soil

No information available.

12.5 Results of PBT and vPvB assessment

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

12.6 Other adverse effects

*Henry constant*

446 Pa*m³/mol

(Lit.) Distribution preferentially in air.

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 2222

14.2 Proper shipping name ANISOLE

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 2222

14.2 Proper shipping name
ANISOLE

14.3 Class
3

14.4 Packing group
III

14.5 Environmentally hazardous
--

14.6 Special precautions for user
no

Sea transport (IMDG)

14.1 UN number
UN 2222

14.2 Proper shipping name
ANISOLE

14.3 Class
3

14.4 Packing group
III

14.5 Environmentally hazardous
--

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 Legislation
SEVESO III 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.

Regulation (EC) No 1005/2009 on substances that deplete the ozone layer
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 \( \geq 0.1 \% \) (w/w).

National legislation
Storage class 3

15.2 Chemical Safety Assessment

A Chemical Safety Assessment has been carried out according to regulation (EC) No. 1907/2006 (REACH) for this substance.

SECTION 16. Other information

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

H226 Flammable liquid and vapour.

Full text of R-phrases referred to under sections 2 and 3

R10 Flammable.

Training advice
Provide adequate information, instruction and training for operators.

Labelling

Hazard pictograms

Signal word
Warning
**Hazard statements**

H226 Flammable liquid and vapour.

**Precautionary statements**

Prevention

P210 Keep away from heat.

**Labelling (67/548/EEC or 1999/45/EC)**

<table>
<thead>
<tr>
<th>R-phrase(s)</th>
<th>S-phrase(s)</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>16-24</td>
<td>Flammable.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Keep away from sources of ignition - No smoking. Avoid contact with skin.</td>
</tr>
</tbody>
</table>

EC-No. 202-876-1

**Reduced labelling (<125 ml)**

<table>
<thead>
<tr>
<th>R-phrase(s)</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>Flammable.</td>
</tr>
</tbody>
</table>

**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.*
EXPOSURE SCENARIO 1 (Industrial use)

1. Industrial use (Chemical for synthesis)

Sectors of end-use

- **SU 3**: Industrial uses: Uses of substances as such or in preparations at industrial sites
- **SU9**: Manufacture of fine chemicals
- **SU 10**: Formulation [mixing] of preparations and/or re-packaging (excluding alloys)

Chemical product category

- **PC19**: Intermediate
- **PC21**: Laboratory chemicals

Process categories

- **PROC1**: Use in closed process, no likelihood of exposure
- **PROC2**: Use in closed, continuous process with occasional controlled exposure
- **PROC3**: Use in closed batch process (synthesis or formulation)
- **PROC4**: Use in batch and other process (synthesis) where opportunity for exposure arises
- **PROC5**: Mixing or blending in batch processes for formulation of preparations and articles (multistage and/or significant contact)
- **PROC8a**: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at non-dedicated facilities
- **PROC8b**: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at dedicated facilities
- **PROC9**: Transfer of substance or preparation into small containers (dedicated filling line, including weighing)
- **PROC10**: Roller application or brushing
- **PROC15**: Use as laboratory reagent

Environmental Release Categories

- **ERC2**: Formulation of preparations
- **ERC4**: Industrial use of processing aids in processes and products, not becoming part of articles
- **ERC6a**: Industrial use resulting in manufacture of another substance (use of intermediates)
- **ERC6b**: Industrial use of reactive processing aids

2. Contributing scenarios: Operational conditions and risk management measures

2.1 Contributing scenario controlling worker exposure for: PROC1
Product characteristics

Concentration of the Substance in Mixture/Article: Covers the percentage of the substance in the product up to 100%.

Physical Form (at time of use): Low volatile liquid

Process Temperature: < 45 °C

Frequency and duration of use

Frequency of use: 8 hours/day

Frequency of use: 5 days/week

Other operational conditions affecting workers exposure

Outdoor / Indoor: Indoor without local exhaust ventilation (LEV)

Organisational measures to prevent/limit releases, dispersion and exposure

Covers daily exposures up to 8 hours.

Conditions and measures related to personal protection, hygiene and health evaluation

Wear suitable gloves tested to EN374. Tightly fitting safety goggles

2.2 Contributing scenario controlling worker exposure for: PROC2, PROC3, PROC4, PROC8b, PROC15

Product characteristics

Concentration of the Substance in Mixture/Article: Covers the percentage of the substance in the product up to 100%.

Physical Form (at time of use): Low volatile liquid

Process Temperature: < 45 °C

Frequency and duration of use

Frequency of use: 8 hours/day

Frequency of use: 5 days/week

Other operational conditions affecting workers exposure

Outdoor / Indoor: Indoor with local exhaust ventilation (LEV)

Organisational measures to prevent/limit releases, dispersion and exposure

Covers daily exposures up to 8 hours.

Conditions and measures related to personal protection, hygiene and health evaluation
Wear suitable gloves tested to EN374. Tightly fitting safety goggles

2.3 Contributing scenario controlling worker exposure for: PROC5, PROC8a, PROC9, PROC10

Product characteristics
- Concentration of the Substance in Mixture/Article: Covers the percentage of the substance in the product up to 100 %.
- Physical Form (at time of use): Low volatile liquid
- Process Temperature: < 45 °C

Frequency and duration of use
- Frequency of use: 8 hours/day
- Frequency of use: 5 days/week

Other operational conditions affecting workers exposure
- Outdoor / Indoor: Indoor with LEV and good general ventilation

Organisational measures to prevent /limit releases, dispersion and exposure
Covers daily exposures up to 8 hours.

Conditions and measures related to personal protection, hygiene and health evaluation
Wear suitable gloves tested to EN374. Tightly fitting safety goggles

3. Exposure estimation and reference to its source

Environment
A chemical safety assessment was performed according REACH Article 14(3), Annex I, sections 3 (Environmental Hazard Assessment) and 4 (PBT/vPvB Assessment). As no hazard was identified, an exposure assessment and risk characterisation is not necessary (REACH Annex I section 5.0).

Workers
<table>
<thead>
<tr>
<th>CS</th>
<th>Use descriptor</th>
<th>Exposure duration, route, effect</th>
<th>RCR</th>
<th>Exposure Assessment Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>PROC1</td>
<td>longterm, inhalative, systemic</td>
<td>&lt; 0,01</td>
<td>ECETOC TRA 3</td>
</tr>
</tbody>
</table>

The Safety Data Sheets for catalogue items are available at www.merckgroup.com
| 2.2 PROC2 | longterm, inhalative, systemic | 0.11 | ECETOC TRA 3 |
| 2.2 PROC3 | longterm, inhalative, systemic | 0.23 | ECETOC TRA 3 |
| 2.2 PROC4 | longterm, inhalative, systemic | 0.45 | ECETOC TRA 3 |
| 2.2 PROC8b | longterm, inhalative, systemic | 0.28 | ECETOC TRA 3 |
| 2.2 PROC15 | longterm, inhalative, systemic | 0.23 | ECETOC TRA 3 |
| 2.3 PROC5 | longterm, inhalative, systemic | 0.79 | ECETOC TRA 3 |
| 2.3 PROC8a | longterm, inhalative, systemic | 0.79 | ECETOC TRA 3 |
| 2.3 PROC9 | longterm, inhalative, systemic | 0.79 | ECETOC TRA 3 |
| 2.3 PROC10 | longterm, inhalative, systemic | 0.79 | ECETOC TRA 3 |

The default parameters and -efficiencies of the applied exposure assessment model were used for the calculation (unless stated differently).

4. Guidance to Downstream User to evaluate whether he works inside the boundaries set by the Exposure Scenario

Please refer to the following documents: ECHA Guidance on information requirements and chemical safety assessment Chapter R.12: Use descriptor system; ECHA Guidance for downstream users; ECHA Guidance on information requirements and chemical safety assessment Part D: Exposure Scenario Building, Part E: Risk Characterisation and Part G: Extending the SDS; VCI/Cefic REACH Practical Guides on Exposure Assessment and Communications in the Supply Chain; CEFIC Guidance Specific Environmental Release Categories (SPERCs).

For scaling of worker exposure assessments performed with ECETOC TRA, please consult the Merck tool ScIDeEx® at www.merckmillipore.com/scideex.
EXPOSURE SCENARIO 2 (Professional use)

1. Professional use (Chemical for synthesis)

Sectors of end-use

SU 22 Professional uses: Public domain (administration, education, entertainment, services, craftsmen)

Chemical product category

PC21 Laboratory chemicals

Process categories

PROC15 Use as laboratory reagent

Environmental Release Categories

ERC8a Wide dispersive indoor use of processing aids in open systems

ERC8b Wide dispersive indoor use of reactive substances in open systems

2. Contributing scenarios: Operational conditions and risk management measures

2.1 Contributing scenario controlling worker exposure for: PROC15

Product characteristics

Concentration of the Substance in Mixture/Article
Covers the percentage of the substance in the product up to 100 %.

Physical Form (at time of use)
Low volatile liquid

Process Temperature
< 45 °C

Frequency and duration of use

Frequency of use 8 hours/day

Frequency of use 5 days/week

Other operational conditions affecting workers exposure

Outdoor / Indoor Indoor with local exhaust ventilation (LEV)

Organisational measures to prevent /limit releases, dispersion and exposure

Covers daily exposures up to 8 hours.

Conditions and measures related to personal protection, hygiene and health evaluation

Wear suitable gloves tested to EN374. Tightly fitting safety goggles
3. Exposure estimation and reference to its source

Environment
A chemical safety assessment was performed according REACH Article 14(3), Annex I, sections 3 (Environmental Hazard Assessment) and 4 (PBT/vPvB Assessment). As no hazard was identified, an exposure assessment and risk characterisation is not necessary (REACH Annex I section 5.0).

Workers

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<tr>
<td>2.1</td>
<td>PROC15</td>
<td>longterm, inhalative, systemic</td>
<td>0.45</td>
<td>ECETOC TRA 3</td>
</tr>
</tbody>
</table>

The default parameters and -efficiencies of the applied exposure assessment model were used for the calculation (unless stated differently).

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