SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 24.03.2016 Version 10.0

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

1.1 Product identifier

Catalogue No.	801452
Product name	Anisole for synthesis
REACH Registration Number	01-2119968918-13-XXXX
CAS-No.	100-66-3

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

Identified uses	Chemical for synthesis In compliance with the conditions described in the annex to this safety data sheet.

1.3 Details of the supplier of the safety data sheet

Company	Merck KGaA * 64271 Darmstadt * Germany * Phone:+49 6151 72-0
Responsible Department	EQ-RS * 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)

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)

Hazard pictograms

Signal word

Warning

CAS-No. 100-66-3

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

Formula	$C_6H_5OCH_3$	C_7H_8O (Hill)
EC-No.	202-876-1	
Molar mass	108,13 g/mol	

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 entrepeneur 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

(External MSDS)

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	SEVESO III
Legislation	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

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

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)

R-phrase(s)	10	Flammable.
S-phrase(s)	16-24	Keep away from sources of ignition - No smoking. Avoid contact with skin.
EC-No.	202-876-1	

Reduced labelling (≤125 ml)

R-phrase(s)	10	Flammable.

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

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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

CS	Use descriptor	Exposure duration, route, effect	RCR	Exposure Assessment Method
2.1	PROC1	longterm, inhalative, systemic	< 0,01	ECETOC TRA 3

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

CS	Use descriptor	Exposure duration, route, effect	RCR	Exposure Assessment Method
2.1	PROC15	longterm, inhalative, systemic	0,45	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.